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LOGINID:ssptasxml624

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	OCT 02	CA/CAPplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	3	OCT 19	BEILSTEIN updated with new compounds
NEWS	4	NOV 15	Derwent Indian patent publication number format enhanced
NEWS	5	NOV 19	WPIX enhanced with XML display format
NEWS	6	NOV 30	ICSD reloaded with enhancements
NEWS	7	DEC 04	LINPADOCDB now available on STN
NEWS	8	DEC 14	BEILSTEIN pricing structure to change
NEWS	9	DEC 17	USPATOLD added to additional database clusters
NEWS	10	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS	11	DEC 17	DGENE now includes more than 10 million sequences
NEWS	12	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS	13	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS	14	DEC 17	CA/CAPplus enhanced with new custom IPC display formats
NEWS	15	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS	16	JAN 02	STN pricing information for 2008 now available
NEWS	17	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	18	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	19	JAN 28	MARPAT searching enhanced
NEWS	20	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	21	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	22	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS	23	FEB 08	STN Express, Version 8.3, now available
NEWS	24	FEB 20	PCI now available as a replacement to DPCI
NEWS	25	FEB 25	IFIREF reloaded with enhancements
NEWS	26	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	27	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,  
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 21:37:07 ON 25 MAR 2008

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 21:37:29 ON 25 MAR 2008

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 MAR 2008 HIGHEST RN 1009867-59-7

DICTIONARY FILE UPDATES: 24 MAR 2008 HIGHEST RN 1009867-59-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

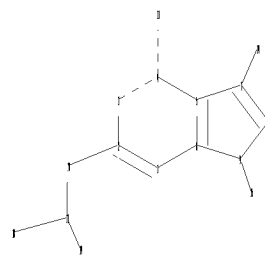
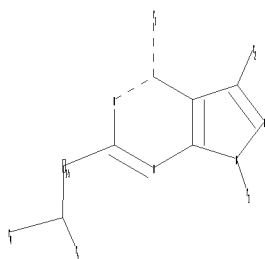
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10524956.str



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10 11 14 15 18 19
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
17
chain bonds :
2-10 4-11 7-14 9-15 10-17 17-18 17-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-11 5-6 5-7 6-9 7-8 7-14 8-9 9-15 17-18 17-19
exact bonds :
2-10 10-17

```

G1:O,S

G2:H,CH3

G3:Cb,Ak

G4:H,Ak,O

G5:H,Ak

G6:H,Ak,OH,O

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 19:CLASS

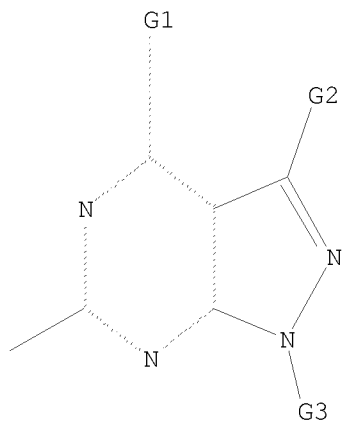
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L1            STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1            STR



G1 O,S

G2 H,Me

G3 Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sam

SAMPLE SEARCH INITIATED 21:37:55 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -        385 TO ITERATE

100.0% PROCESSED        385 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*

BATCH    \*\*COMPLETE\*\*

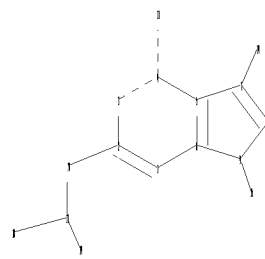
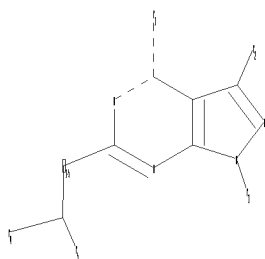
PROJECTED ITERATIONS:        6523 TO        8877

PROJECTED ANSWERS:            1367 TO        2553

L2            50 SEA SSS SAM L1

=>

Uploading C:\Program Files\Stnexp\Queries\10524956.str



```

chain nodes :
10 11 14 15 18 19
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
17
chain bonds :
2-10 4-11 7-14 9-15 10-17 17-18 17-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-11 5-6 5-7 6-9 7-8 7-14 8-9 9-15 17-18 17-19
exact bonds :
2-10 10-17

```

G1:O,S

G2:H,CH3

G3:Cb,Ak

G4:H,Ak,O

G5:H,Ak

G6:H,Ak,OH,O

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 19:CLASS

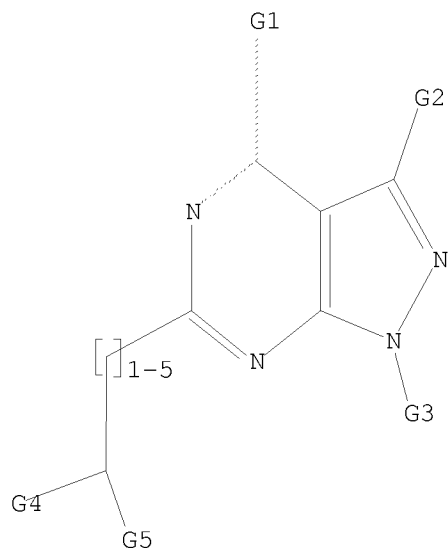
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L3            STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3            STR



G1 O, S

G2 H, Me

G3 Cb, Ak

G4 H, Ak, O

G5 H, Ak

G6 H, Ak, OH, O

Structure attributes must be viewed using STN Express query preparation.

=> s 13 sam

SAMPLE SEARCH INITIATED 21:42:42 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -        118 TO ITERATE

100.0% PROCESSED        118 ITERATIONS

22 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                              BATCH    \*\*COMPLETE\*\*

PROJECTED ITERATIONS:        1709 TO        3011

PROJECTED ANSWERS:            159 TO        721

L4            22 SEA SSS SAM L3

=> s 13 full

FULL SEARCH INITIATED 21:42:50 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -        2014 TO ITERATE

100.0% PROCESSED      2014 ITERATIONS  
SEARCH TIME: 00.00.01

331 ANSWERS

L5                    331 SEA SSS FUL L3

=> fil capl

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

182.04

182.25

FILE 'CAPLUS' ENTERED AT 21:43:04 ON 25 MAR 2008

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FILE COVERS 1907 - 25 Mar 2008 VOL 148 ISS 13

FILE LAST UPDATED: 24 Mar 2008 (20080324/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 15

L6                    27 L5

=> s 16 not (2008/so or 2007/so or 2006/so or 2005/so or 2004/so)

151404 2008/SO

894006 2007/SO

936349 2006/SO

882724 2005/SO

849072 2004/SO

L7                    24 L6 NOT (2008/SO OR 2007/SO OR 2006/SO OR 2005/SO OR 2004/SO)

=> d 17 ibib hitstr abs 1-24

L7 ANSWER 1 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:729227 CAPLUS

DOCUMENT NUMBER: 147:143456

TITLE: Fused pyrimidones and thiopyrimidones, and their preparation, pharmaceutical compositions and use in killing or reducing cancer cell proliferation

INVENTOR(S): Venkat, Raj Gopal; Qi, Longwu; Pierce, Michael; Robbins, Paul B.; Sahasrabudhe, Sudhir R.; Selliah, Robert

PATENT ASSIGNEE(S): Prolexys Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 77pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007076085	A2	20070705	WO 2006-US49168	20061222
WO 2007076085	A3	20070823		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			

PRIORITY APPLN. INFO.: US 2005-753916P P 20051222  
US 2006-834989P P 20060727

OTHER SOURCE(S): MARPAT 147:143456

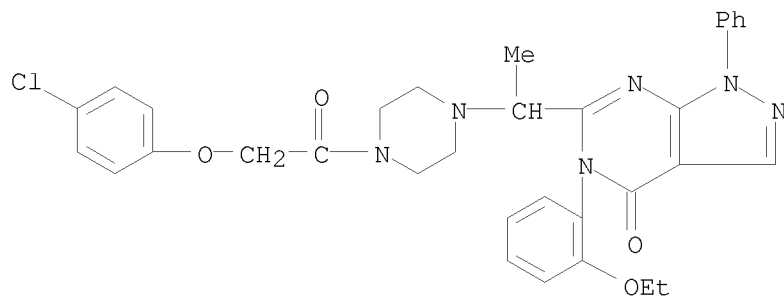
IT 943431-00-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of fused pyrimidone and thiopyrimidone compds. useful in killing or reducing cancer cell proliferation)

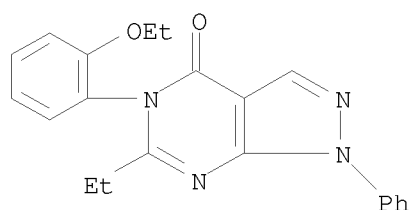
RN 943431-00-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[1-[4-[2-(4-chlorophenoxy)acetyl]-1-piperazinyl]ethyl]-5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl- (CA INDEX NAME)

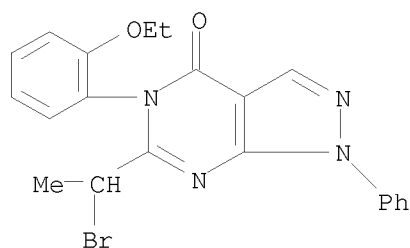




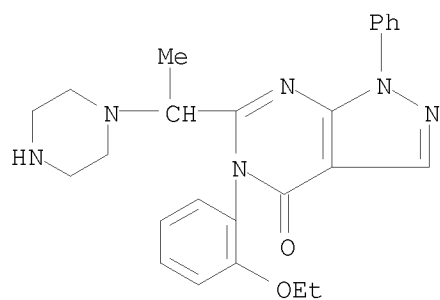
IT 943431-16-1P 943431-17-2P 943431-18-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (intermediate; preparation of fused pyrimidone and thiopyrimidone compds.  
 useful in killing or reducing cancer cell proliferation)  
 RN 943431-16-1 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-(2-ethoxyphenyl)-6-ethyl-1,5-dihydro-  
 1-phenyl- (CA INDEX NAME)



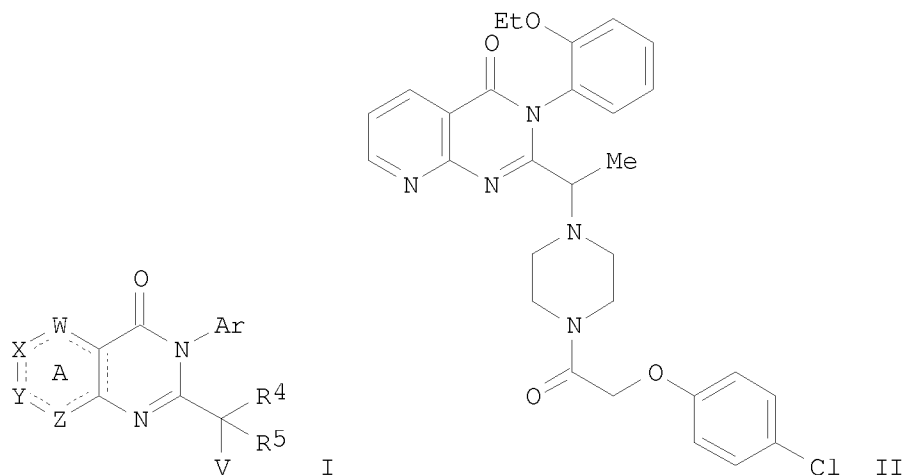
RN 943431-17-2 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(1-bromoethyl)-5-(2-ethoxyphenyl)-1,5-  
 dihydro-1-phenyl- (CA INDEX NAME)



RN 943431-18-3 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl-  
 6-[1-(1-piperazinyl)ethyl]- (CA INDEX NAME)



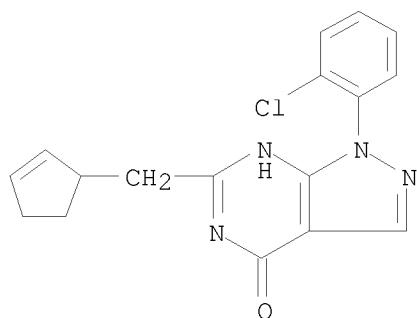
GI



AB Comps. represented by structural formula I: are useful, for example, in the effective killing or reduction in rate of proliferation of cancer cells, such as in patients suffering from cancer. In addition to the comps. themselves, the invention provides pharmaceutical compns. of the comps. and method of treatment using the comps. Comps. of formula I wherein ring A is optionally substituted: W is absent, C, N, S and O; X, Y and Z is C, N, S and O where at least one of X, Y and Z is N if W is C; Ar is (un)substituted phenyl; R4 and R5 are independently H, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted heterocyclyl, and (un)substituted aryl; V is substituted amine and cyclic amines; dotted lines are single and double bonds; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by a general procedure. All the invention comps. were evaluated for their ability to kill or reduce cancer cell proliferation.

L7 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:1253041 CAPLUS  
 DOCUMENT NUMBER: 146:757  
 TITLE: Use of pyrazolopyrimidine compounds for the treatment of cardiovascular diseases  
 INVENTOR(S): Hendrix, Martin; Wunder, Frank; Tersteegen, Adrian; Stasch, Johannes-Peter  
 PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany  
 SOURCE: PCT Int. Appl., 48pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006125548	A1	20061130	WO 2006-EP4591	20060516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102005024493	A1	20061130	DE 2005-102005024493	20050527
EP 1888076	A1	20080220	EP 2006-753634	20060516
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRIORITY APPLN. INFO.:			DE 2005-102005024493A	20050527
			WO 2006-EP4591	W 20060516
OTHER SOURCE(S): MARPAT 146:757				
IT 794568-65-3				
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pyrazolopyrimidine compds. for treatment of cardiovascular diseases)				
RN 794568-65-3 CAPLUS				
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro- (CA INDEX NAME)				



AB The invention discloses the use of pyrazolopyrimidine compds. for  
producing medicaments drugs for treating cardiovascular diseases.  
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:471917 CAPLUS  
DOCUMENT NUMBER: 144:488675  
TITLE: Preparation of 1,4-substituted pyrazolopyrimidines as  
kinase inhibitors, particularly EphB4 inhibitors  
INVENTOR(S): Schmiedeberg, Niko; Furet, Pascal; Imbach, Patricia;  
Holzer, Philipp  
PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma GmbH  
SOURCE: PCT Int. Appl., 88 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006050946	A1	20060518	WO 2005-EP12045	20051110
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AU 2005303965	A1	20060518	AU 2005-303965	20051110
CA 2585660	A1	20060518	CA 2005-2585660	20051110
EP 1812441	A1	20070801	EP 2005-819276	20051110
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CN 101098873	A	20080102	CN 2005-80046410	20051110
IN 2007DN03269	A	20070831	IN 2007-DN3269	20070501
MX 200705644	A	20070605	MX 2007-5644	20070510
KR 2007084191	A	20070824	KR 2007-710778	20070511
PRIORITY APPLN. INFO.:			GB 2004-25035	A 20041112
			WO 2005-EP12045	W 20051110

OTHER SOURCE(S): MARPAT 144:488675

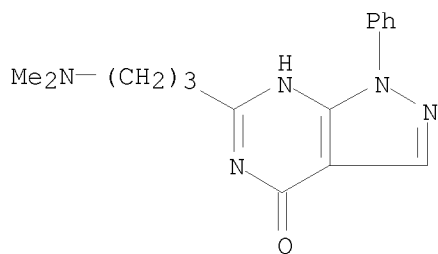
IT 887327-53-9P, 6-(3-Dimethylaminopropyl)-1-phenyl-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

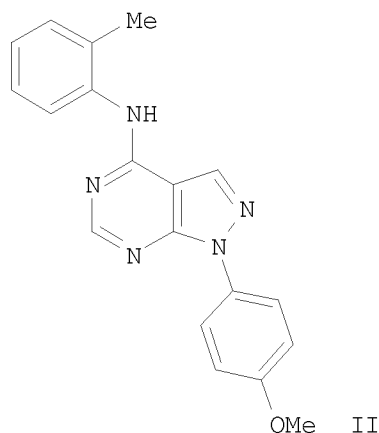
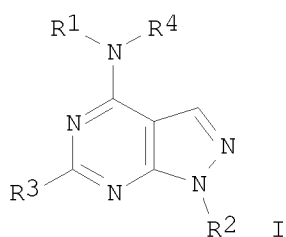
(intermediate; preparation of 1,4-substituted pyrazolopyrimidines as EphB4 inhibitors)

RN 887327-53-9 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[3-(dimethylamino)propyl]-1,5-dihydro-1-phenyl- (CA INDEX NAME)



GI



AB The invention is related to 1,4-substituted pyrazolopyrimidines I [R1 = (un)substituted Ph; R2 = (un)substituted aryl; R3 = H, (un)substituted alkyl, aryl, heterocyclyl; R4 = H, (un)substituted alkyl], and their pharmaceutically acceptable salts where one or more salt-forming groups are present, pharmaceuticals comprising them, and their use in the diagnosis and treatment or manufacture of a pharmaceutical formulation for the treatment of a disease that depends on inadequate activity of a protein kinase, especially a protein tyrosine kinase, preferably one or more of c-Abl, c-Src and/or especially Ephrin B4 receptor (EphB4) kinases; and/or one or more altered or mutated forms of any one or more of these, e.g. those forms that result in conversion of the resp. proto-oncogene into an oncogene, such as constitutively activated Bcr-Abl or v-Src. The invention is also related to the preparation of pyrazolopyrimidines I. Thus, II•TFA was

prepared starting from 4-methoxyphenylhydrazine•xHCl and  
(ethoxymethylene)malononitrile. Pyrazolopyrimidine II•TFA inhibited  
EphB4 (Ic50 = 0.16  $\mu$ mol/l).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:979639 CAPLUS  
DOCUMENT NUMBER: 143:286443  
TITLE: Preparation of pyrimidine derivatives as 5-HT3  
receptor antagonists having agonistic activity on  
5-HT1A  
INVENTOR(S): Sato, Michitaka; Matsui, Teruaki; Asagarasu, Akira;  
Hayashi, Hiroyuki; Araki, Seiichi; Tamaoki, Satoru;  
Takahashi, Nobuyuki; Yamauchi, Yukinao; Yamamoto,  
Yoshiko; Yamamoto, Norio; Ogawa, Chisato  
PATENT ASSIGNEE(S): Teikoku Hormone Mfg. Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 261 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005082887	A1	20050909	WO 2005-JP3691	20050225
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005217320	A1	20050909	AU 2005-217320	20050225
CA 2557541	A1	20050909	CA 2005-2557541	20050225
EP 1724267	A1	20061122	EP 2005-719969	20050225
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1922171	A	20070228	CN 2005-80005603	20050225
US 2007197551	A1	20070823	US 2006-590707	20060825
PRIORITY APPLN. INFO.:			JP 2004-52040	A 20040226
			JP 2004-322858	A 20041105
			WO 2005-JP3691	W 20050225

OTHER SOURCE(S): MARPAT 143:286443

IT 864386-94-7P

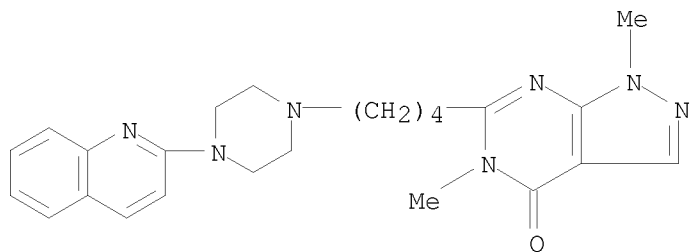
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of pyrimidine derivs. as 5-HT3 receptor antagonists having  
agonistic activity on 5-HT1A for treatment of anxiety, depression,  
etc.)

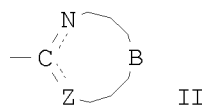
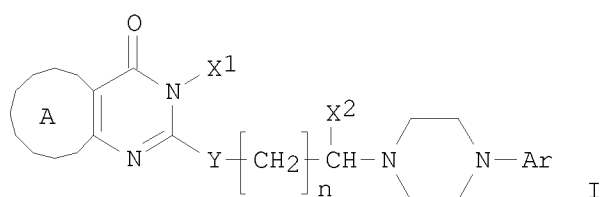
RN 864386-94-7 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,5-dimethyl-6-[4-[4-(2-  
quinolinyl)-1-piperazinyl]butyl]- (CA INDEX NAME)





GI



AB Title compds. I [ring A = carbocyclic group, etc.; X1 = H, amino, etc.; X2 = H, alkyl; Y = bond, etc.; n = 0-4; Ar = optionally substituted II with halo, etc.; Z = O, etc.; B = moiety required for completing mono-, ploy-heterocyclic ring containing N together with N-C-Z; dotted line indicates single, double bond] were prepared For example, treatment of potassium 3-amino-5,6-dimethyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidine-2-thiolate with 2-[4-(3-chloropropyl)piperazin-1-yl]quinoline, e.g., prepared from piperazine in 2 steps, afforded 3-amino-5,6-dimethyl-2-[3-(4-quinolin-2-ylpiperazin-1-yl)propylthio]-3H-thieno[2,3-d]pyrimidin-4-one (III) in 50% yield. In 5-HT3 receptor affinity assay (in vitro), compound III exhibited the antagonistic activity of 94% at 10<sup>-7</sup> M. Compds. I are claimed useful for the treatment of anxiety, depression, etc. Formulation is given.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:238744 CAPLUS  
DOCUMENT NUMBER: 142:316851  
TITLE: Preparation of fused ring heterocycles as potassium channel modulators  
INVENTOR(S): McNaughton-Smith, Grant Andrew; Amato, George Salvatore; Thomas, James Barnwell  
PATENT ASSIGNEE(S): Icagen, Inc., USA  
SOURCE: U.S. Pat. Appl. Publ., 39 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005059823	A1	20050317	US 2004-937958	20040910
US 7223768	B2	20070529		
AU 2004272104	A1	20050324	AU 2004-272104	20040910
CA 2536633	A1	20050324	CA 2004-2536633	20040910
WO 2005025293	A2	20050324	WO 2004-US29868	20040910
WO 2005025293	A3	20050616		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1663237	A2	20060607	EP 2004-788717	20040910
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
JP 2007505143	T	20070308	JP 2006-526375	20040910
US 2008058319	A1	20080306	US 2007-740831	20070426
PRIORITY APPLN. INFO.:			US 2003-502109P	P 20030910
			US 2004-937958	A1 20040910
			WO 2004-US29868	W 20040910

OTHER SOURCE(S): CASREACT 142:316851; MARPAT 142:316851

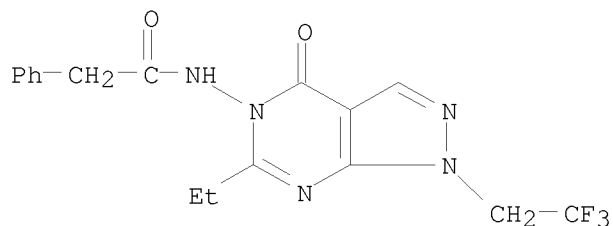
IT 848027-62-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

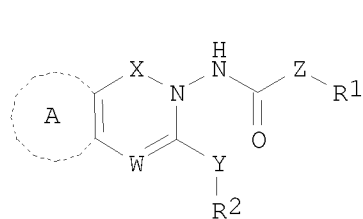
(preparation of quinazolines as potassium channel modulators)

RN 848027-62-3 CAPLUS

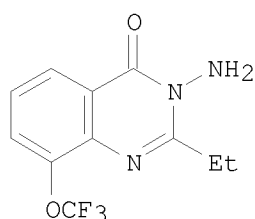
CN Benzeneacetamide, N-[6-ethyl-1,4-dihydro-4-oxo-1-(2,2,2-trifluoroethyl)-5H-pyrazolo[3,4-d]pyrimidin-5-yl]- (CA INDEX NAME)



GI



I



II

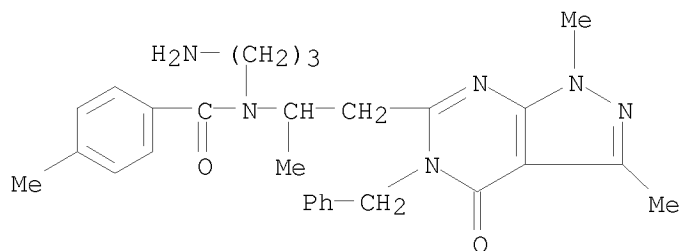
AB Compds. I [A = (un)substituted 5-6 membered (hetero)aryl, cycloalkyl, 5-8 membered heteroaryl; X = CO, CS, SO<sub>2</sub>; W = N, CR<sub>3</sub> (wherein R<sub>3</sub> = H, F, (un)substituted (hetero)aryl, etc.); Z = a bond, CH<sub>2</sub>, CHF, CH:CH, etc.; Y = (CR<sub>5</sub>R<sub>6</sub>)<sub>n</sub> (n = 0-4; R<sub>5</sub>, R<sub>6</sub> = H, F, (un)substituted (hetero)aryl, etc.); R<sub>1</sub> = (un)substituted (hetero)aryl, cycloalkyl, 5-7 membered heterocyclyl, alkyl; R<sub>2</sub> = CF<sub>3</sub>, (un)substituted alkyl, (hetero)aryl, cycloalkyl, 3-7 membered heterocyclyl], compns. and methods are provided which are useful in the treatment of diseases through the modulation of potassium ion flux through voltage-dependent potassium channels. More particularly, the invention provides quinazolinones, compns. and methods that are useful in the treatment of central or peripheral nervous system disorders (e.g., migraine, ataxia, Parkinson's disease, bipolar disorders, trigeminal neuralgia, spasticity, mood disorders, brain tumors, psychotic disorders, myokymia, seizures, epilepsy, hearing and vision loss, Alzheimer's disease, age-related memory loss, learning deficiencies, anxiety and motor neuron diseases, maintaining bladder control or treating urinary incontinence) and as neuroprotective agents (e.g., to prevent stroke and the like) by modulating potassium channels associated with the onset or recurrence of the indicated conditions. E.g., a multi-step synthesis of II, starting from 2-trifluoromethoxyaniline, was given. The compound II and analogs were subsequently coupled with isocyanates and carboxylic acids to provide the compds. I such as 1-(2-cyclohexyl-4-oxo-4H-quinazolin-3-yl)-3-(2-fluorobenzyl)urea. The representative compds. I were tested for the ability to open voltage-gated potassium channels in the NG-108-15 FLIPR assay (data given for selected compds. I).

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

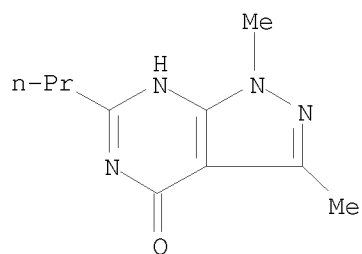
ACCESSION NUMBER: 2004:1038663 CAPLUS  
DOCUMENT NUMBER: 142:6555  
TITLE: Preparation of bicyclic pyrimidones as Eg5 modulators  
for treatment of cancer  
INVENTOR(S): Kim, Kyoung S.; Lu, Songfeng; Sheng, X. Christopher;  
Crews, Alvin Donald  
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA  
SOURCE: U.S. Pat. Appl. Publ., 39 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004242596	A1	20041202	US 2004-848089	20040518
US 7022850	B2	20060404		
WO 2004106492	A2	20041209	WO 2004-US15972	20040521
WO 2004106492	A3	20050519		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1628981	A2	20060301	EP 2004-752900	20040521
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR			
PRIORITY APPLN. INFO.:			US 2003-472880P	P 20030522
			WO 2004-US15972	W 20040521
OTHER SOURCE(S):	MARPAT 142:6555			
IT 799295-87-7P				
RL:	PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)			
	(anticancer agent; preparation of bicyclic pyrimidones as Eg5 modulators for treatment of cancer)			
RN 799295-87-7 CAPLUS				
CN	Benzamide, N-(3-aminopropyl)-N-[2-[4,5-dihydro-1,3-dimethyl-4-oxo-5-(phenylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-1-methylethyl]-4-methyl-, monohydrochloride (9CI) (CA INDEX NAME)			

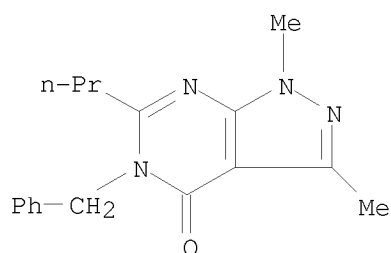


● HCl

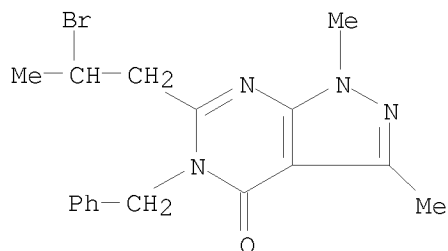
IT 799295-88-8P, 1,3-Dimethyl-6-propyl-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-4-one 799295-89-9P, 1,3-Dimethyl-5-benzyl-6-propyl-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-4-one 799295-90-2P, 1,3-Dimethyl-5-benzyl-6-( $\alpha$ -bromopropyl)-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-4-one 799295-91-3P, 1,3-Dimethyl-5-benzyl-6-[2-[[3-[(tert-butoxycarbonyl)amino]propyl]amino]propyl]-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-4-one  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of bicyclic pyrimidones as Eg5 modulators for treatment of cancer)  
 RN 799295-88-8 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,3-dimethyl-6-propyl- (CA INDEX NAME)



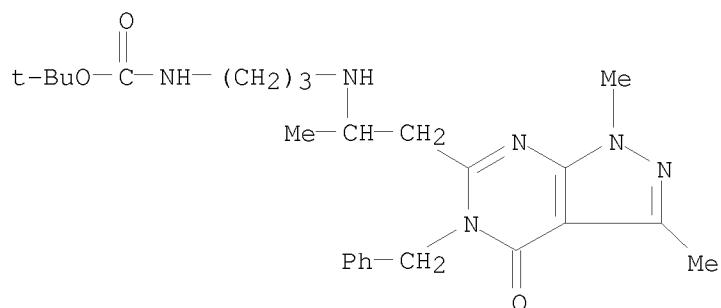
RN 799295-89-9 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,3-dimethyl-5-(phenylmethyl)-6-propyl- (CA INDEX NAME)



RN 799295-90-2 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-bromopropyl)-1,5-dihydro-1,3-dimethyl-5-(phenylmethyl)- (CA INDEX NAME)



RN 799295-91-3 CAPLUS  
 CN Carbamic acid, [3-[[2-[4,5-dihydro-1,3-dimethyl-4-oxo-5-(phenylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-1-methylethyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title isoxazolopyrimidinones, pyrazolopyrimidinones, and isothiazolopyrimidinones I or II [wherein X = O, S, N; provided that if X = O or S, then Y2 is absent; Y1 = H, (un)substituted (cyclo)alkyl, aryl; Y2 = absent, H, alkyl; Z = O, X; R1 = H, (un)substituted alkyl, aryl, (hetero)arylalkyl; R2, R3 = independently H, (cyclo)alkyl, halo; or CR2R3 = cycloalkyl; n = 1, 2; A = N; R4 = COR9, CO2R10, CONR11R12, SO2R13, (un)substituted (cyclo)alkyl, (hetero)aryl; R5, R9-R13 = independently H, (un)substituted (cyclo)alkyl, (hetero)aryl] were prepared as Eg5 modulators (no data). I and II induce mitotic arrest, thereby making them useful as anticancer agents. For example, cycloaddn. of 2-(1-ethoxyethylidene)malononitrile and hydroxylamine•HCl gave 5-amino-3-methylisoxazole-4-carbonitrile (72%), which was coupled with butyric anhydride to provide 3-methyl-6-propyl-5H-isoxazolo[5,4-d]pyrimidin-4-one (52%). The isoxazol[5,4-d]pyrimidin-4-one was then benzylated (20%), brominated (30%), aminated with 1,3-diaminopropane (66%), acylated with 4-toluoyl chloride (95%), and deprotected (65%) to afford III. Compds. of the invention exhibited activity in a 72-h cell

proliferation assay, inhibiting cell proliferation against one or more of ovarian, breast, prostate, lung, leukemia, or colorectal human cancer cell lines with IC50 values  $\leq 10 \mu\text{M}$ . I and II also exhibited activity in a clonogenicity assay and a cell cycle profile anal. assay, producing significant increases in mitotic and apoptotic fractions of the cell population. Addnl., invention compds. inhibited bipolar spindle formation and induced a monoastal array of microtubules in immunocytochem. assays. Thus, I, II, and their pharmaceutical compns., optionally in combination with at least one other anticancer agent, are useful for the treatment of cancer and other proliferative disorders.

L7 ANSWER 7 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:996183 CAPLUS  
DOCUMENT NUMBER: 141:424206  
TITLE: Preparation of pyrazolopyrimidinones as  
phosphodiesterase 9A inhibitors useful as nootropics.  
INVENTOR(S): Hendrix, Martin; Baerfacker, Lars; Erb, Christina;  
Hafner, Frank-Thorsten; Heckroth, Heike; Schauss,  
Dagmar; Tersteegen, Adrian; Van Der Staay,  
Franz-Josef; Van Kampen, Marja  
PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany  
SOURCE: PCT Int. Appl., 96 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004099211	A1	20041118	WO 2004-EP4455	20040428
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 102004004142	A1	20041125	DE 2004-102004004142	20040128
AU 2004235915	A1	20041118	AU 2004-235915	20040428
CA 2524900	A1	20041118	CA 2004-2524900	20040428
EP 1626971	A1	20060222	EP 2004-729876	20040428
R: DE, ES, FR, GB, IT				
JP 2006525966	T	20061116	JP 2006-505294	20040428
US 2007105876	A1	20070510	US 2005-556224	20051109
IN 2005DN05418	A	20070928	IN 2005-DN5418	20051124
PRIORITY APPLN. INFO.:			DE 2003-10320784	A 20030509
			DE 2003-10336183	A 20030807
			DE 2004-102004004142A	20040128
			WO 2004-EP4455	W 20040428

OTHER SOURCE(S): MARPAT 141:424206

IT 794568-84-6P 794568-87-9P 794568-90-4P

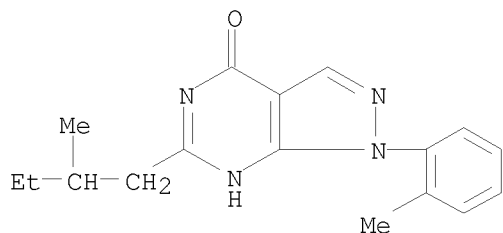
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)

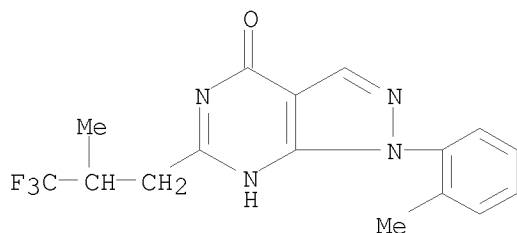
RN 794568-84-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(2-methylbutyl)-1-(2-methylphenyl)- (CA INDEX NAME)

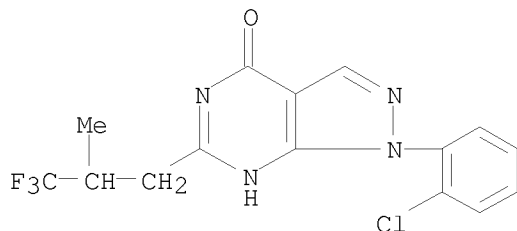




RN 794568-87-9 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-(3,3,3-trifluoro-2-methylpropyl)- (CA INDEX NAME)

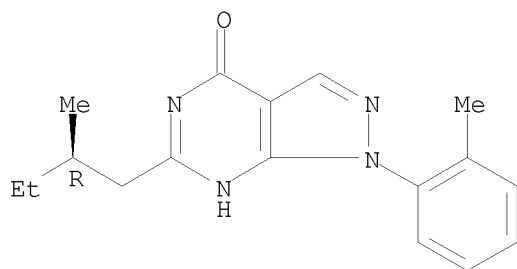


RN 794568-90-4 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-(3,3,3-trifluoro-2-methylpropyl)- (CA INDEX NAME)



IT 794568-85-7P 794568-86-8P 794568-88-0P  
 794568-89-1P 794568-91-5P 794568-92-6P  
 RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)  
 RN 794568-85-7 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(2R)-2-methylbutyl]-1-(2-methylphenyl)- (CA INDEX NAME)

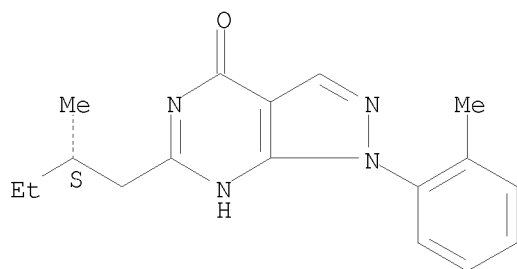
Absolute stereochemistry.



RN 794568-86-8 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(2S)-2-methylbutyl]-1-(2-methylphenyl)- (CA INDEX NAME)

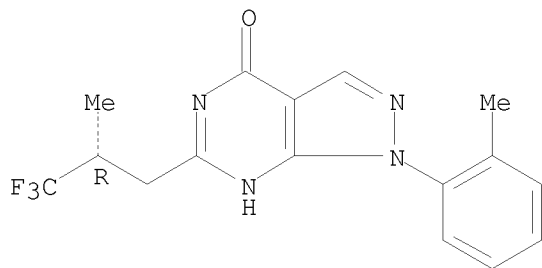
Absolute stereochemistry.



RN 794568-88-0 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

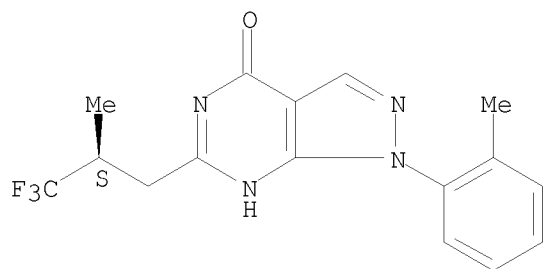
Absolute stereochemistry.



RN 794568-89-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-[(2S)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

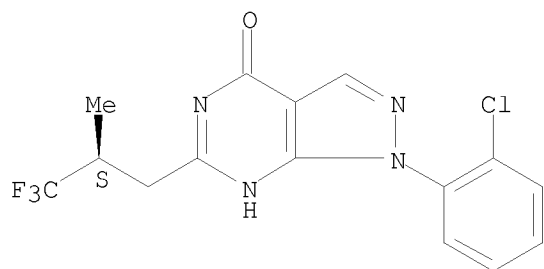
Absolute stereochemistry.



RN 794568-91-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-[(2S)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

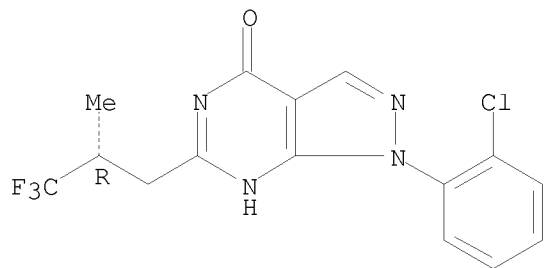
Absolute stereochemistry.



RN 794568-92-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 794568-50-6P 794568-51-7P 794568-52-8P  
 794568-53-9P 794568-54-0P 794568-55-1P  
 794568-56-2P 794568-57-3P 794568-58-4P  
 794568-59-5P 794568-60-8P 794568-61-9P  
 794568-62-0P 794568-63-1P 794568-64-2P  
 794568-65-3P 794568-67-5P 794568-68-6P  
 794568-69-7P 794568-70-0P 794568-71-1P  
 794568-72-2P 794568-73-3P 794568-74-4P  
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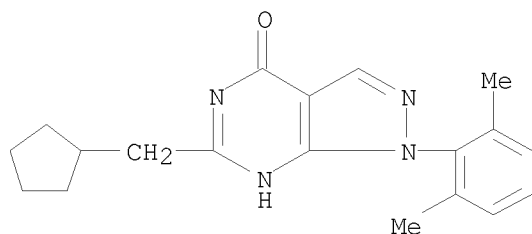
794568-83-5P 794568-97-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)

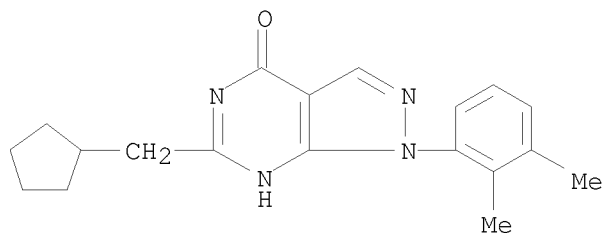
RN 794568-50-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,6-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



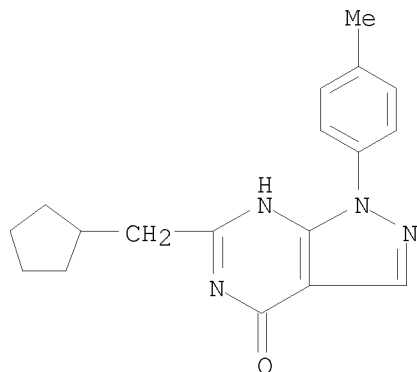
RN 794568-51-7 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,3-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



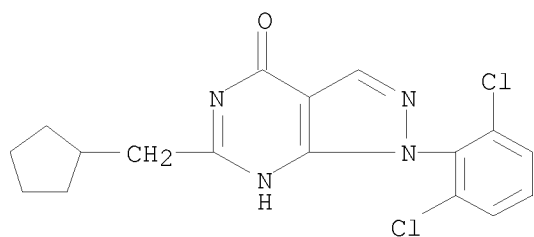
RN 794568-52-8 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methylphenyl)- (CA INDEX NAME)



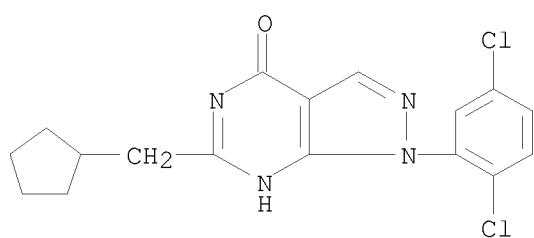
RN 794568-53-9 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,6-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



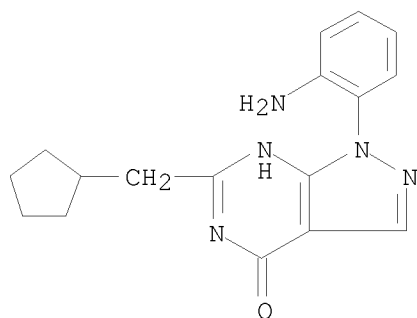
RN 794568-54-0 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,5-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



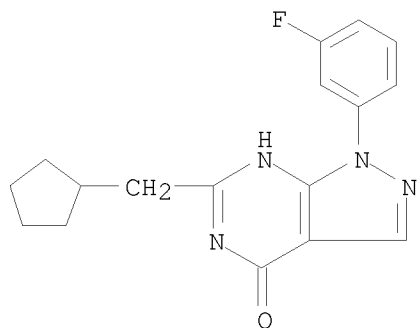
RN 794568-55-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-aminophenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)



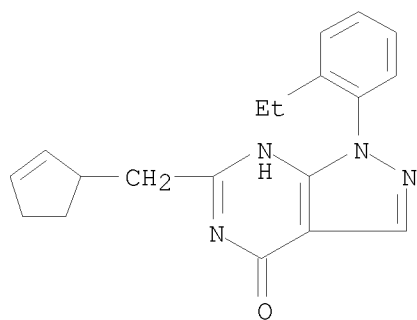
RN 794568-56-2 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(3-fluorophenyl)-1,5-dihydro- (CA INDEX NAME)



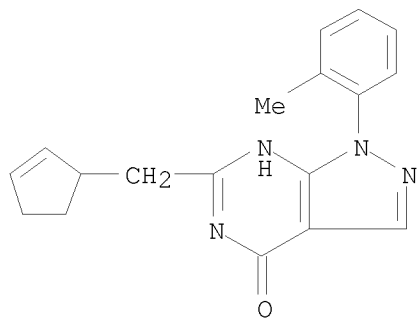
RN 794568-57-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1-(2-ethylphenyl)-1,5-dihydro- (CA INDEX NAME)



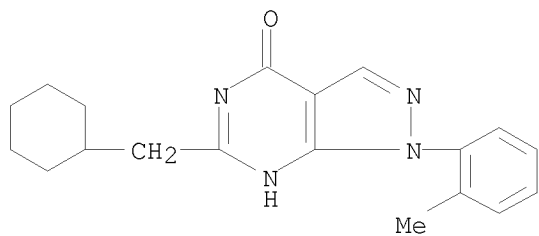
RN 794568-58-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)

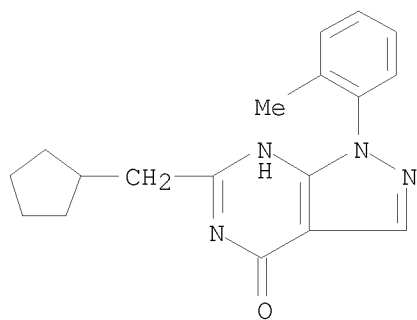


RN 794568-59-5 CAPLUS

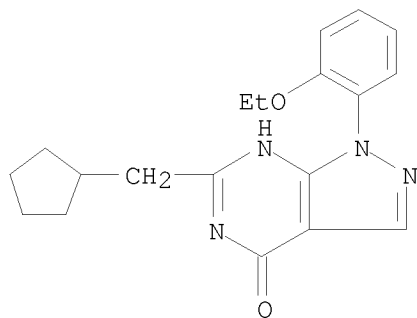
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



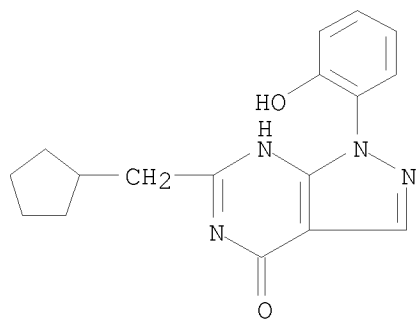
RN 794568-60-8 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



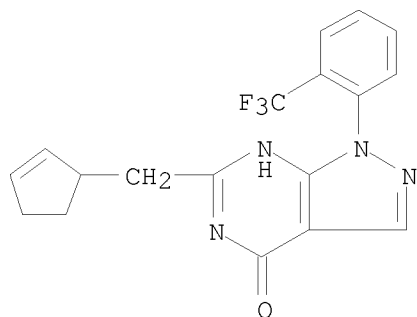
RN 794568-61-9 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2-ethoxyphenyl)-1,5-dihydro- (CA INDEX NAME)



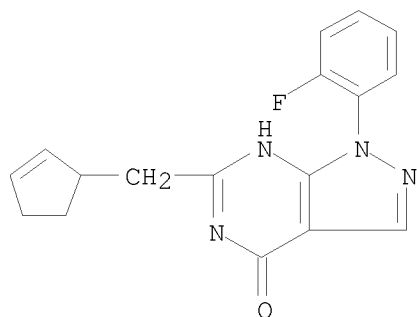
RN 794568-62-0 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(2-hydroxyphenyl)- (CA INDEX NAME)



RN 794568-63-1 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)

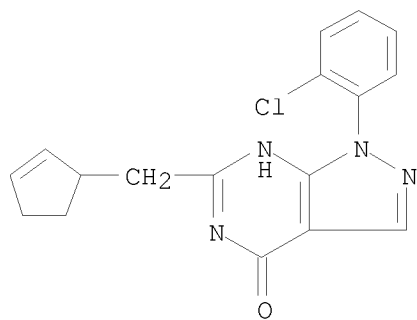


RN 794568-64-2 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1-(2-fluorophenyl)-1,5-dihydro- (CA INDEX NAME)

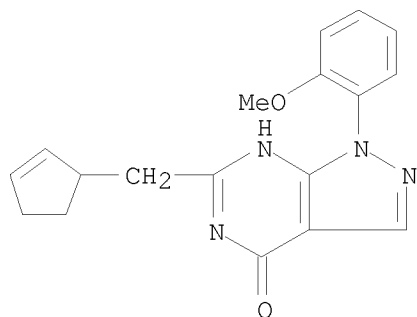


RN 794568-65-3 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro- (CA INDEX NAME)

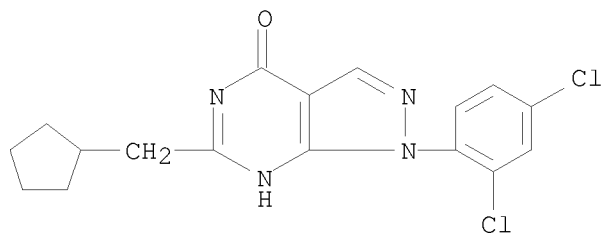




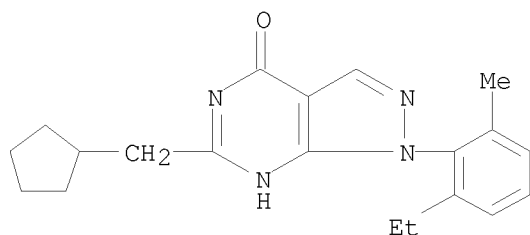
RN 794568-67-5 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-methoxyphenyl)- (CA INDEX NAME)



RN 794568-68-6 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,4-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)

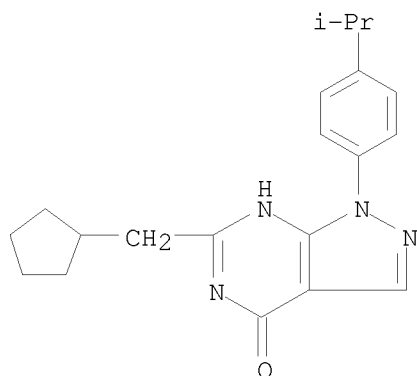


RN 794568-69-7 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2-ethyl-6-methylphenyl)-1,5-dihydro- (CA INDEX NAME)



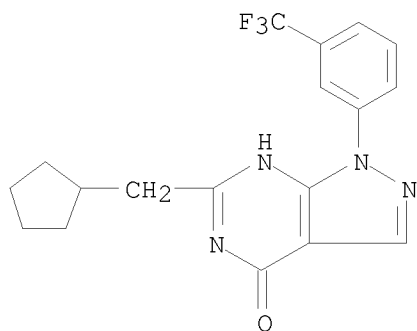
RN 794568-70-0 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



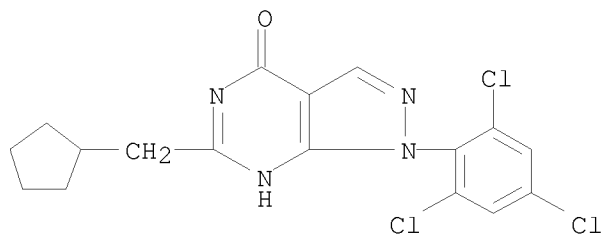
RN 794568-71-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



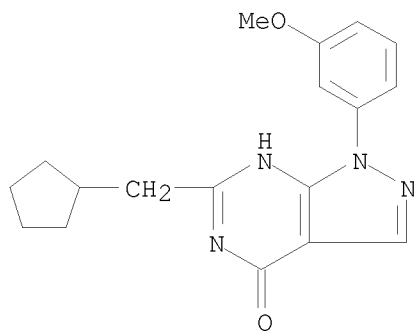
RN 794568-72-2 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



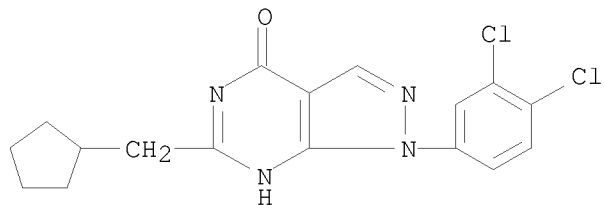
RN 794568-73-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(3-methoxyphenyl)- (CA INDEX NAME)



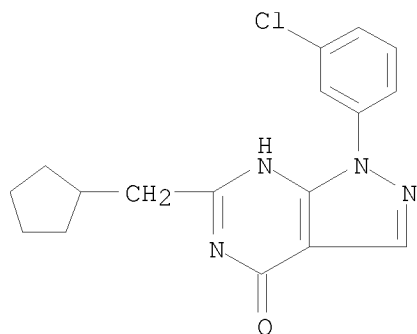
RN 794568-74-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(3,4-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



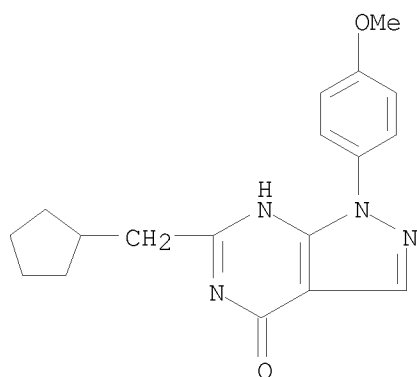
RN 794568-75-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(3-chlorophenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)



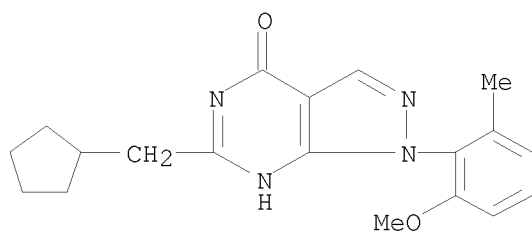
RN 794568-76-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methoxyphenyl)- (CA INDEX NAME)



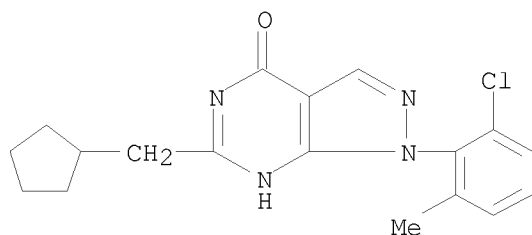
RN 794568-79-9 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(2-methoxy-6-methylphenyl)- (CA INDEX NAME)

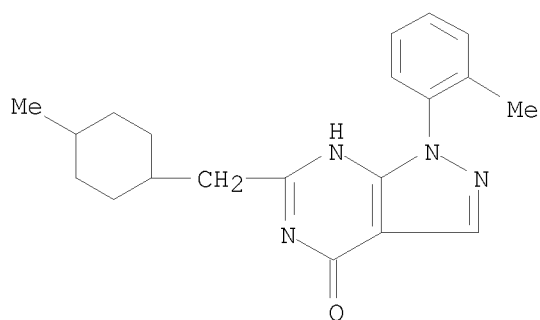


RN 794568-80-2 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chloro-6-methylphenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)

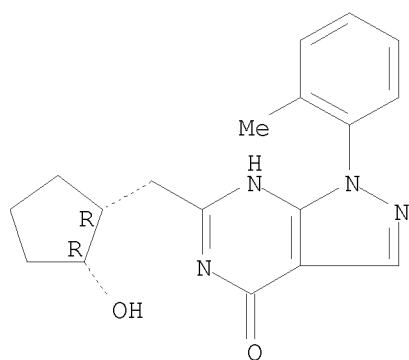


RN 794568-81-3 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(4-methylcyclohexyl)methyl]-1-(2-methylphenyl)- (CA INDEX NAME)



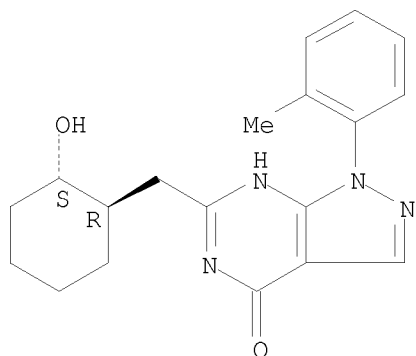
RN 794568-82-4 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[[2-(2-methylphenyl)-2-hydroxycyclopentyl]methyl]-1-(2-methylphenyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.



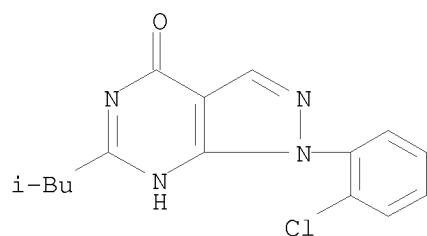
RN 794568-83-5 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[[2-(2-methylphenyl)-2-hydroxycyclohexyl]methyl]-1-(2-methylphenyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.

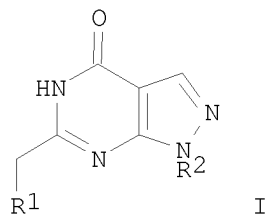


RN 794568-97-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-(2-methylpropyl)- (CA INDEX NAME)



GI



AB Title compds. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = (substituted) Ph, heteroaryl], were prepared Thus, reflux of 5-amino-1-(2-methylphenyl)-1H-pyrazole-4-carboxamide (preparation given) with Et cyclopentylacetate and NaH in EtOH overnight gave 30% 6-cyclopentylmethyl-1-(2-methylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one. The latter inhibited PDE9A with IC50 = 5 nM.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:198173 CAPLUS  
DOCUMENT NUMBER: 140:247085  
TITLE: Selective phosphodiesterase 9A inhibitors for the improvement of cognitive processes  
INVENTOR(S): Boss, Frank-Gerhard; Erb, Christina; Hendrix, Martin; Van Kampen, Marja; Wunder, Frank  
PATENT ASSIGNEE(S): Bayer AG, Germany  
SOURCE: Ger. Offen., 17 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10238722	A1	20040311	DE 2002-10238722	20020823
CA 2496292	A1	20040401	CA 2003-2496292	20030811
WO 2004026286	A2	20040401	WO 2003-EP8880	20030811
WO 2004026286	A3	20040603		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003258597	A1	20040408	AU 2003-258597	20030811
EP 1534285	A2	20050601	EP 2003-797233	20030811
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 2006501272	T	20060112	JP 2004-536933	20030811
US 2006100222	A1	20060511	US 2005-525119	20051014
PRIORITY APPLN. INFO.:			DE 2002-10238722	A 20020823
			WO 2003-EP8880	W 20030811

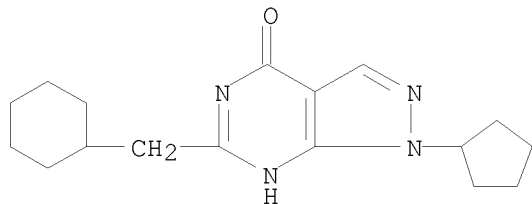
IT 667400-78-4P 667400-79-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(phosphodiesterase 9A inhibitors for improvement of cognitive processes)

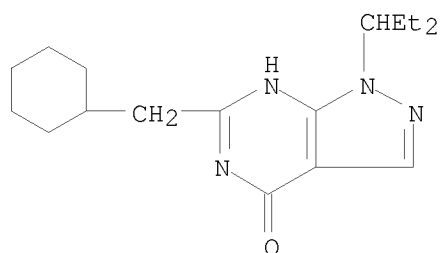
RN 667400-78-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



RN 667400-79-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1-(1-ethylpropyl)-  
1,5-dihydro- (CA INDEX NAME)



AB The invention discloses the use of selective phosphodiesterase 9A inhibitors for the production of drugs for the improvement of perception, concentration, cognitive processes, learning and/or memory. Preparation and activity of pyrazolopyrimidinone derivs. is included.



L7 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:177919 CAPLUS  
DOCUMENT NUMBER: 140:235735  
TITLE: Preparation of pyrazolopyrimidines as  
phosphodiesterase PDE9A inhibitors.  
INVENTOR(S): Hendrix, Martin; Boess, Frank-Gerhard; Burkhardt,  
Nils; Erb, Christina; Tersteegen, Adrian; Van Kampen,  
Marja  
PATENT ASSIGNEE(S): Bayer A.-G., Germany  
SOURCE: Ger. Offen., 28 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10238724	A1	20040304	DE 2002-10238724	20020823
CA 2496308	A1	20040401	CA 2003-2496308	20030813
WO 2004026876	A1	20040401	WO 2003-EP8979	20030813
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003251706	A1	20040408	AU 2003-251706	20030813
EP 1534713	A1	20050601	EP 2003-797239	20030813
EP 1534713	B1	20060111		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 2006503051	T	20060126	JP 2004-536941	20030813
ES 2256797	T3	20060716	ES 2003-797239	20030813
US 2006111372	A1	20060525	US 2005-524956	20051215
PRIORITY APPLN. INFO.:			DE 2002-10238724	A 20020823
			WO 2003-EP8979	W 20030813

OTHER SOURCE(S): MARPAT 140:235735

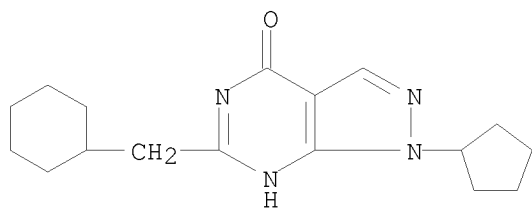
IT 667400-78-4P 667400-79-5P 667870-10-2P  
667870-11-3P 667870-12-4P 667870-13-5P  
667870-14-6P 667870-15-7P 667870-16-8P  
667870-17-9P 667870-18-0P 667870-19-1P  
667870-20-4P 667870-21-5P 667870-22-6P  
667870-23-7P 667870-24-8P 667870-25-9P  
667870-26-0P 667870-27-1P 667870-28-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of pyrazolopyrimidines as phosphodiesterase PDE9A inhibitors.)

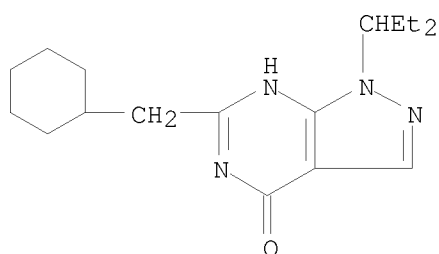
RN 667400-78-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



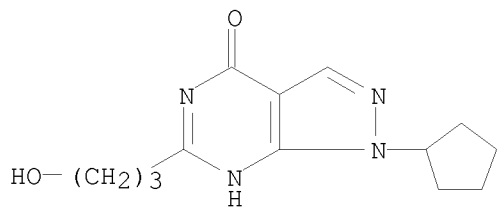
RN 667400-79-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1-(1-ethylpropyl)-1,5-dihydro- (CA INDEX NAME)



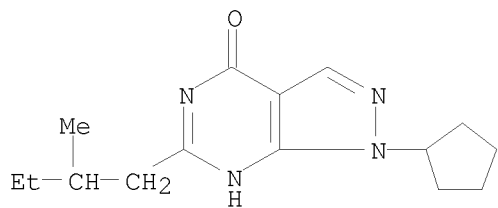
RN 667870-10-2 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-(3-hydroxypropyl)- (CA INDEX NAME)



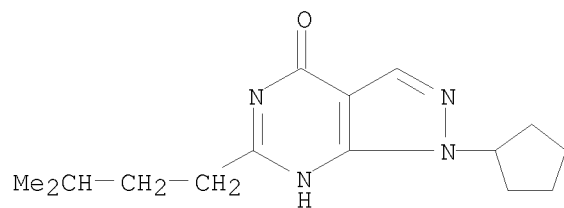
RN 667870-11-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-(2-methylbutyl)- (CA INDEX NAME)



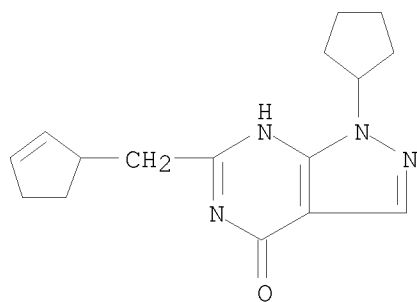
RN 667870-12-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-(3-methylbutyl)- (CA INDEX NAME)



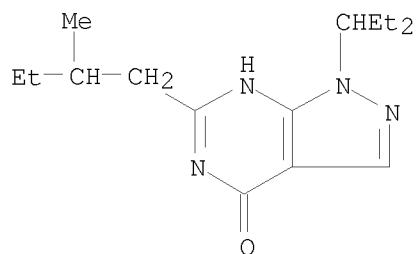
RN 667870-13-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



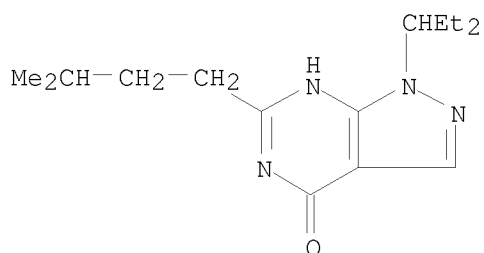
RN 667870-14-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylpropyl)-1,5-dihydro-6-(2-methylbutyl)- (CA INDEX NAME)

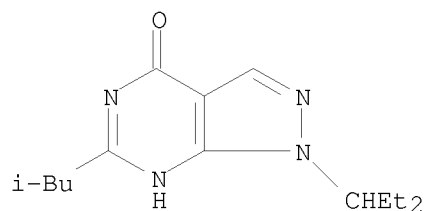


RN 667870-15-7 CAPLUS

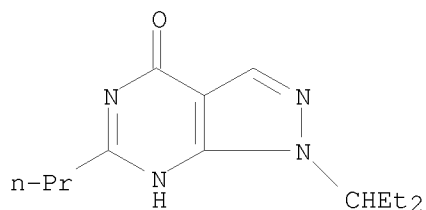
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylpropyl)-1,5-dihydro-6-(3-methylbutyl)- (CA INDEX NAME)



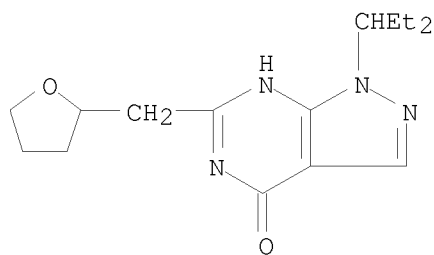
RN 667870-16-8 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylpropyl)-1,5-dihydro-6-(2-methylpropyl)- (CA INDEX NAME)



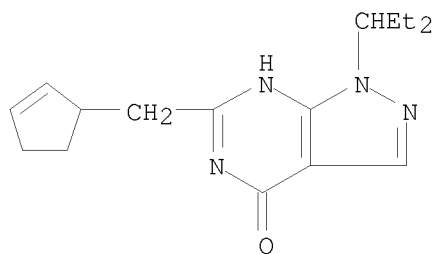
RN 667870-17-9 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylpropyl)-1,5-dihydro-6-propyl- (CA INDEX NAME)



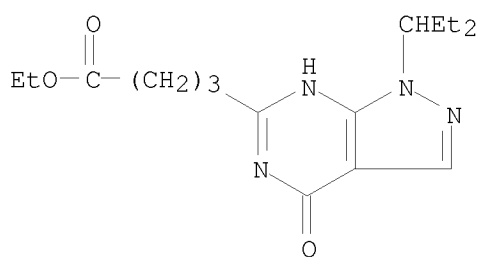
RN 667870-18-0 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylpropyl)-1,5-dihydro-6-[(tetrahydro-2-furanyl)methyl]- (CA INDEX NAME)



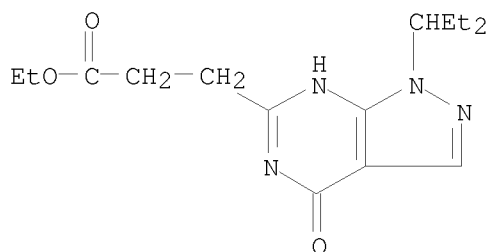
RN 667870-19-1 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1-(1-ethylpropyl)-1,5-dihydro- (CA INDEX NAME)



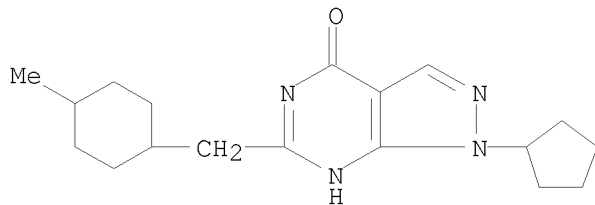
RN 667870-20-4 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-6-butanoic acid, 1-(1-ethylpropyl)-4,5-dihydro-4-oxo-, ethyl ester (CA INDEX NAME)



RN 667870-21-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanoic acid, 1-(1-ethylpropyl)-4,5-dihydro-4-oxo-, ethyl ester (CA INDEX NAME)

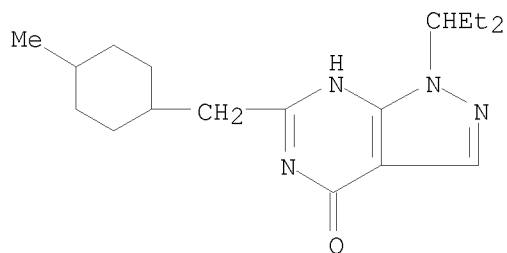


RN 667870-22-6 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[(4-methylcyclohexyl)methyl]- (CA INDEX NAME)



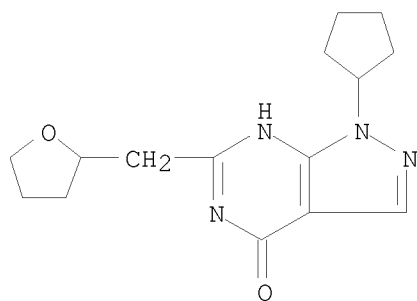
RN 667870-23-7 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylpropyl)-1,5-dihydro-6-[(4-methylcyclohexyl)methyl]- (CA INDEX NAME)



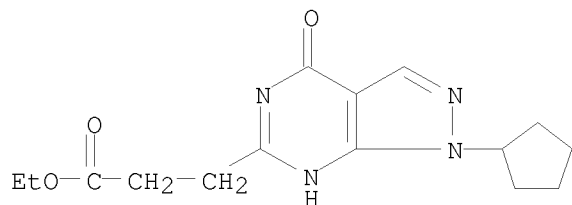
RN 667870-24-8 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[(tetrahydro-2-furanyl)methyl]- (CA INDEX NAME)



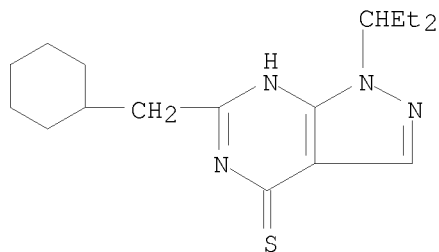
RN 667870-25-9 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanoic acid, 1-cyclopentyl-4,5-dihydro-4-oxo-, ethyl ester (CA INDEX NAME)

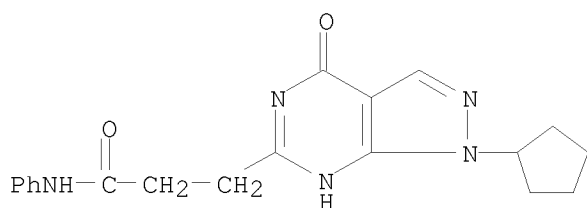


RN 667870-26-0 CAPLUS

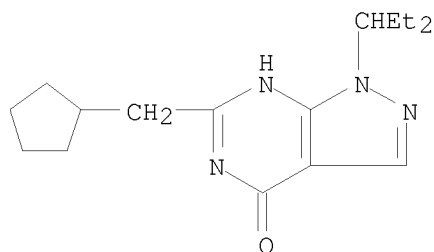
CN 4H-Pyrazolo[3,4-d]pyrimidine-4-thione, 6-(cyclohexylmethyl)-1-(1-ethylpropyl)-1,5-dihydro- (CA INDEX NAME)



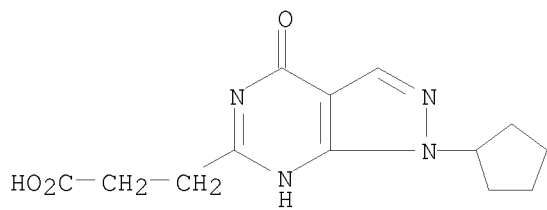
RN 667870-27-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanamide, 1-cyclopentyl-4,5-dihydro-4-oxo-N-phenyl- (CA INDEX NAME)



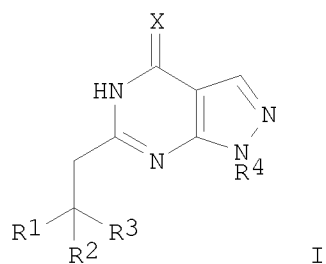
RN 667870-28-2 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(1-ethylpropyl)-1,5-dihydro- (CA INDEX NAME)



IT 667870-31-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of pyrazolopyrimidines as phosphodiesterase PDE9A inhibitors.)  
 RN 667870-31-7 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanoic acid, 1-cyclopentyl-4,5-dihydro-4-oxo- (CA INDEX NAME)



GI



AB Title compds. [I; R1 = OH, (substituted) alkyl, alkoxy, CO2R5, CONR6R7; R5 = alkyl; R6, R7 = H, aryl, alkyl; NR6R7 = 4-10 membered heterocycle; R2 = H, alkyl, alkoxy; R3 = H, alkyl; R4 = pentan-3-yl, C4-6 cycloalkyl; X = O, S], were prepared Thus, 5-amino-1-cyclopentyl-1H-pyrazole-4-carboxamide (preparation given), Me cyclohexylacetate, and NaH were refluxed 18 h in EtOH to give 31% 6-cyclohexylmethyl-1-cyclopentyl-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one. The latter inhibited PDE9A with IC50 = 5 nM.



L7 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:891929 CAPLUS  
DOCUMENT NUMBER: 139:381500  
TITLE: Preparation of pyrazolo[3,4-d]pyrimidin-4-ones as herbicides and/or nematocides  
INVENTOR(S): Linker, Karl-Heinz; Andree, Roland; Hoischen, Dorothee; Schwarz, Hans-Georg; Drewes, Mark Wilhelm; Dahmen, Peter; Feucht, Dieter; Pontzen, Rolf; Loesel, Peter  
PATENT ASSIGNEE(S): Bayer CropScience AG, Germany  
SOURCE: Ger. Offen., 36 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10219435	A1	20031113	DE 2002-10219435	20020502
IN 2003MU00379	A	20050211	IN 2003-MU379	20030417
CA 2484997	A1	20031113	CA 2003-2484997	20030422
WO 2003093269	A2	20031113	WO 2003-EP4137	20030422
WO 2003093269	A3	20040408		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003224111	A1	20031117	AU 2003-224111	20030422
EP 1504005	A2	20050209	EP 2003-720510	20030422
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2003009873	A	20050426	BR 2003-9873	20030422
JP 2005531549	T	20051020	JP 2004-501408	20030422
US 2005209251	A1	20050922	US 2005-512834	20050519
PRIORITY APPLN. INFO.:			DE 2002-10219435	A 20020502
			WO 2003-EP4137	W 20030422

OTHER SOURCE(S): MARPAT 139:381500

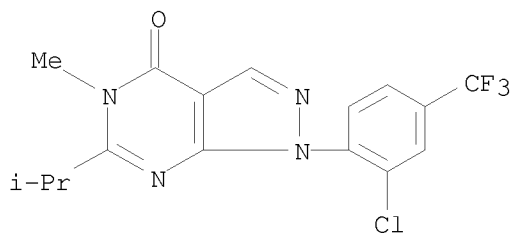
IT 623584-98-5P 623584-99-6P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

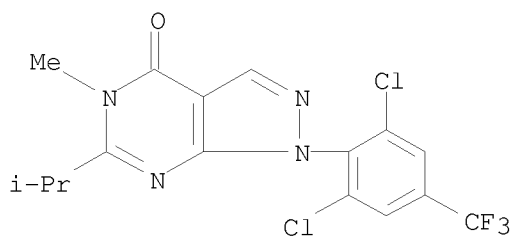
(preparation of pyrazolopyrimidinones as herbicides and/or nematocides)

RN 623584-98-5 CAPLUS

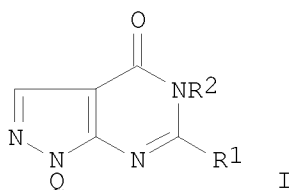
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2-chloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



RN 623584-99-6 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)

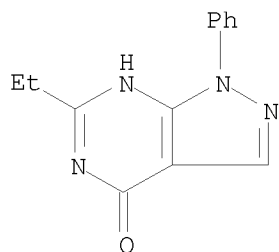


GI

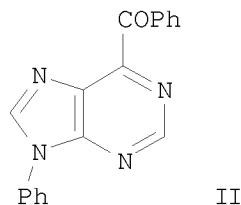


AB Title compds. [I; Q = NO<sub>2</sub>, cyano, halo, (halogenated) alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, (hetero)aryl; R<sub>1</sub> = H, (substituted) alkyl, alkoxy, carbonyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, heterocyclyl; R<sub>2</sub> = H, (substituted) alkyl, alkenyl, alkynyl], were prepared Thus, a mixture of 5-amino-1-(3-chloro-5-trifluoromethylpyridin-2-yl)pyrazole-4-carboxamide, CH(OMe)<sub>3</sub>, p-toluenesulfonic acid, and toluene was refluxed for 12 h followed by further addition of CH(OMe)<sub>3</sub> and reflux for 12 h under stirring to give 44% 1-(3-chloro-5-trifluoromethylpyridin-2-yl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one. I were said to show very strong pre- and postemergent herbicidal activity, good crop tolerance, and good nematocidal activity.

ACCESSION NUMBER: 1998:226504 CAPLUS  
 DOCUMENT NUMBER: 128:282737  
 TITLE: Catalytic action of azolium salts. IX. Synthesis of 6-aroyle-9H-purines and their analogs by nucleophilic aroylation catalyzed by imidazolium or benzimidazolium salt  
 AUTHOR(S): Miyashita, Akira; Suzuki, Yumiko; Iwamoto, Ken-Ichi; Higashino, Takeo  
 CORPORATE SOURCE: School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka, 422, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1998), 46(3), 390-399  
 CODEN: CPBTAL; ISSN: 0009-2363  
 PUBLISHER: Pharmaceutical Society of Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 128:282737  
 IT 5394-42-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis of 6-aroyle-9H-purines and analogs via nucleophilic aroylation catalyzed by imidazolium or benzimidazolium salt)  
 RN 5394-42-3 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



GI



AB In the presence of 1,3-dimethylimidazolium iodide (I), 6-chloro-9-phenyl-9H-purine and 4-chloro-5,6-dimethylpyrrolo[2,3-d]pyrimidines underwent nucleophilic aroylation with arenecarbaldehydes to give the corresponding fused aroylpyrimidines, e.g. II. 1,3-Dimethylbenzimidazolium iodide (III) was an effective catalyst for the similar synthesis of 7-aroyle-3-phenyl-3H-1,2,3-triazolo[4,5-d]pyrimidines. In the synthesis of 4-aroyle-1H-pyrazolo[3,4-d]pyrimidines, both azolium salts I and III were effective as catalysts. Moreover,

4-aroysl-7H-pyrrolo[2,3-d]pyrimidines were obtained in good yields via the 4-tosyl derivs., in the presence of catalytic amts. of sodium p-toluenesulfinate and the imidazolium salt I. This catalytic aroylation was found to be a facile and useful method for the synthesis of 6-aroysl-9H-purines and their analogs.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 12 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:174107 CAPLUS

DOCUMENT NUMBER: 116:174107

TITLE: Versatile synthesis of 6-alkyl(aryl)-1H-pyrazolo[3,4-d]pyrimidin-4[5H]-ones

AUTHOR(S): Reddy, K. Hemender; Reddy, A. Panduranga; Veeranagaiah, V.

CORPORATE SOURCE: Nizam Coll., Osmania Univ., Hyderabad, 500 001, India

SOURCE: Indian Journal of Chemistry, Section B: Organic

Chemistry Including Medicinal Chemistry (1992),

31B(3), 163-6

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 116:174107

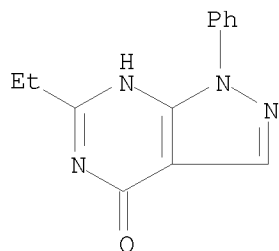
IT 5394-42-3P 130925-64-3P 130925-68-7P

139954-52-2P 139954-53-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

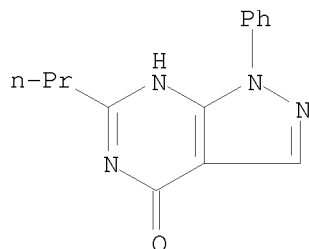
RN 5394-42-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA  
INDEX NAME)



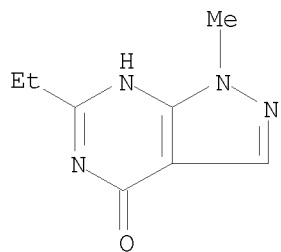
RN 130925-64-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-propyl- (CA  
INDEX NAME)

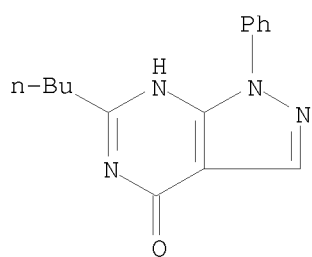


RN 130925-68-7 CAPLUS

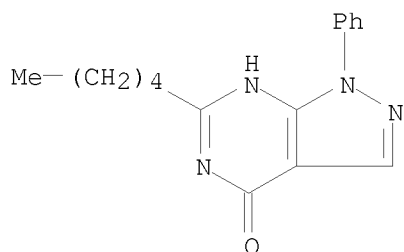
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-methyl- (CA  
INDEX NAME)



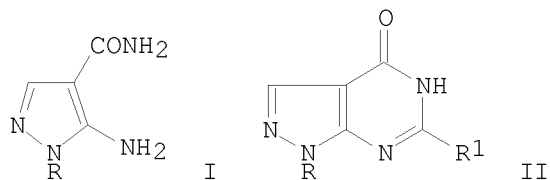
RN 139954-52-2 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-butyl-1,5-dihydro-1-phenyl- (CA  
 INDEX NAME)



RN 139954-53-3 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-pentyl-1-phenyl- (CA  
 INDEX NAME)



GI



AB Condensation of 5-amino-1H-pyrazole-4-carboxamide (I, R = H) with various  
 aromatic aldehydes furnishes 6-substituted 1H-pyrazolo[3,4-d]pyrimidin-4(5H)-  
 ones II (R1 = Ph, substituted Ph) via the intermediate

5-(N-arylideneamino)pyrazole-4-carboxamides. II were also synthesized by the reaction of I (R = H) with aromatic carboxylic acids in polyphosphoric acid (PPA) or polyphosphate ester (PPE). Similar treatment of I (R = Ph, Me) with aromatic aldehydes and aromatic carboxylic acids gives exclusively 6-substituted 1-methyl/phenyl-1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones. The title compds. have were also synthesized by the reaction of I with arylideneanilines.

L7 ANSWER 13 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:6429 CAPLUS

DOCUMENT NUMBER: 114:6429

TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives.  
XVIII. Facile preparation of 1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones

AUTHOR(S): Miyashita, Akira; Iijima, Chihoko; Higashino, Takeo; Matsuda, Hideaki

CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan

SOURCE: Heterocycles (1990), 31(7), 1309-14

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:6429

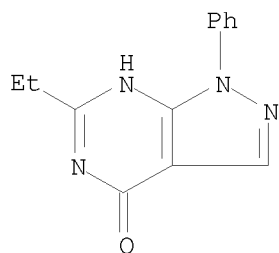
IT 5394-42-3P 130925-64-3P 130925-65-4P

130925-68-7P 130925-69-8P 130925-70-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

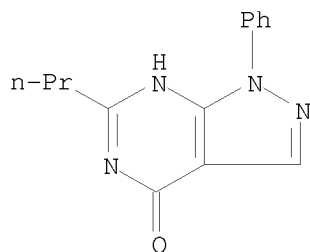
RN 5394-42-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA  
INDEX NAME)



RN 130925-64-3 CAPLUS

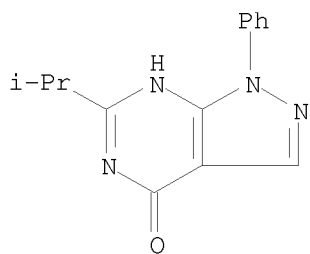
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-propyl- (CA  
INDEX NAME)



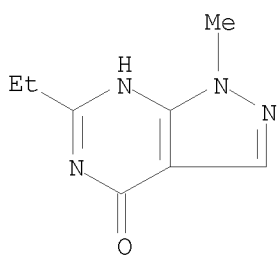
RN 130925-65-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(1-methylethyl)-1-phenyl-  
(CA INDEX NAME)

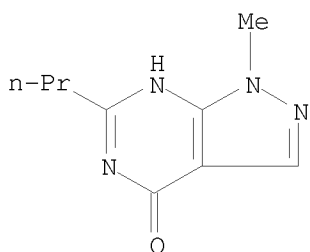




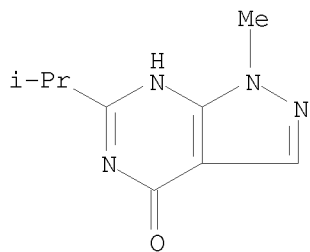
RN 130925-68-7 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-methyl- (CA  
 INDEX NAME)



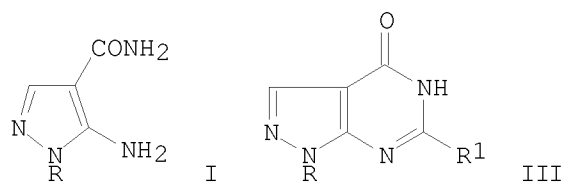
RN 130925-69-8 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-propyl- (CA  
 INDEX NAME)



RN 130925-70-1 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-(1-methylethyl)-  
 (CA INDEX NAME)

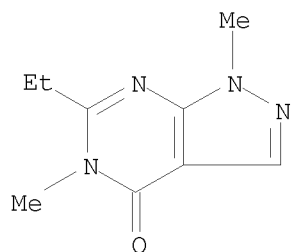


GI

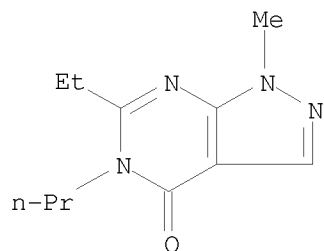


AB     Reaction of 5-amino-1-phenyl-1H-pyrazole-4-carboxamide (I, R = Ph) with  $R_1CO_2R_2$  (II,  $R_1$  = H, Me, Et, Pr,  $Me_2CH$ ,  $PhCH_2$ ,  $CO_2Et$ , Ph;  $R_2$  = Me, Et) in the presence of EtONa-EtOH gave 1-phenylpyrazolopyrimidinones III (R = Ph). Similar treatment of I (R = Me) with II gave III (R = Me).

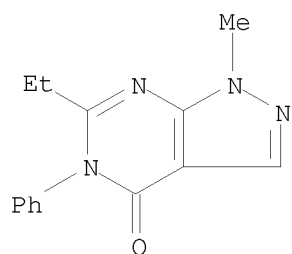
ACCESSION NUMBER: 1984:34489 CAPLUS  
 DOCUMENT NUMBER: 100:34489  
 ORIGINAL REFERENCE NO.: 100:5351a,5354a  
 TITLE: Phosphorus pentoxide in organic synthesis. V.  
 Phosphorus pentoxide and amine hydrochlorides as  
 reagents in the synthesis of 1,5-dihydro-1-methyl-4H-  
 pyrazolo[3,4-d]pyrimidin-4-ones  
 AUTHOR(S): Finlander, Peter; Nielsen, Soeren V.; Pedersen, Erik  
 B.  
 CORPORATE SOURCE: Dep. Chem., Odense Univ., Odense, DK-5230, Den.  
 SOURCE: Chemica Scripta (1983), 22(4), 171-6  
 CODEN: CSRPB9; ISSN: 0004-2056  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 100:34489  
 IT 88320-62-1P 88320-63-2P 88320-64-3P  
 88320-65-4P 88320-66-5P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological  
 study); PREP (Preparation)  
 (preparation and antitumor activity of)  
 RN 88320-62-1 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1,5-dimethyl- (CA  
 INDEX NAME)



RN 88320-63-2 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-methyl-5-propyl-  
 (CA INDEX NAME)

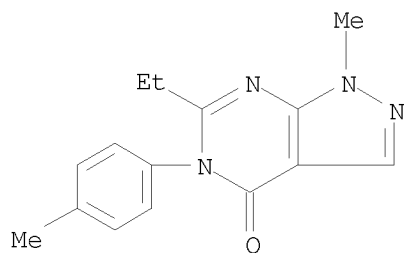


RN 88320-64-3 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-methyl-5-phenyl-  
 (CA INDEX NAME)



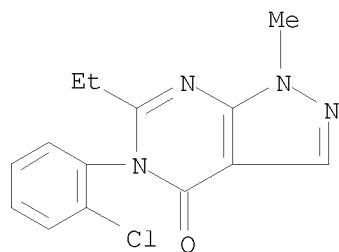
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CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-methyl-5-(4-methylphenyl)- (CA INDEX NAME)

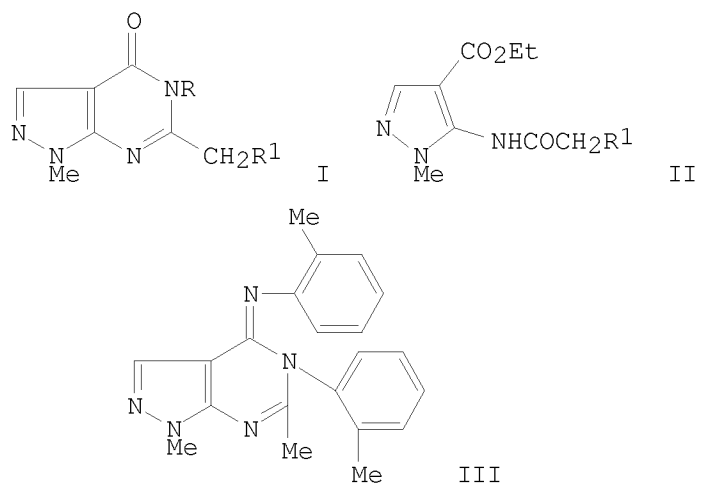


RN 88320-66-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-(2-chlorophenyl)-6-ethyl-1,5-dihydro-1-methyl- (CA INDEX NAME)



GI



AB    Pyrazolo[3,4-d]pyrimidinones I (R = H, alkyl, allyl, CH<sub>2</sub>Ph, Ph, substituted Ph; R<sub>1</sub> = H, Me) were prepared by heating pyrazolecarboxylates II with P<sub>2</sub>O<sub>5</sub>, N,N-dimethylcyclohexylamine and RNH<sub>2</sub>.HCl. When 2-MeC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>.HCl was used it was also possible to isolate III. The results from pesticide and anticancer screenings are given.

L7 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:567969 CAPLUS

DOCUMENT NUMBER: 87:167969

ORIGINAL REFERENCE NO.: 87:26547a,26550a

TITLE: Synthesis of condensed heterocyclic systems of pyrazole

AUTHOR(S): Alonso, G.; Madronero, R.; Nebreda, L.

CORPORATE SOURCE: Inst. Quim. Med., Madrid, Spain

SOURCE: Anales de Quimica (1968-1979) (1976), 72(11-12), 897-901

CODEN: ANQUBU; ISSN: 0365-4990

DOCUMENT TYPE: Journal

LANGUAGE: Spanish

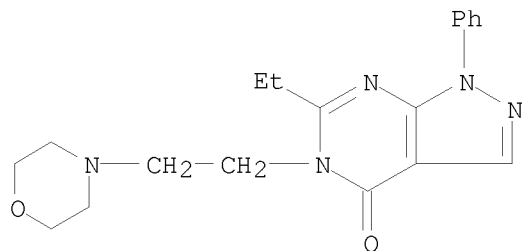
IT 64257-08-5P 64257-09-6P 64257-10-9P

64257-17-6P 64257-19-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

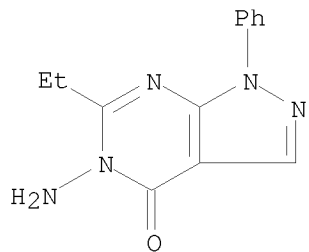
RN 64257-08-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-5-[2-(4-morpholinyl)ethyl]-1-phenyl- (CA INDEX NAME)



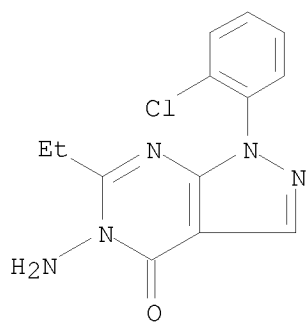
RN 64257-09-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-amino-6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)

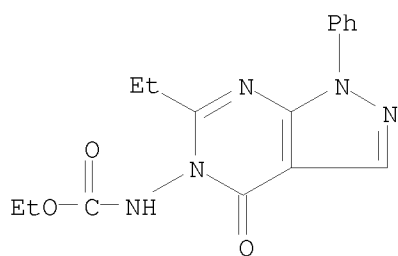


RN 64257-10-9 CAPLUS

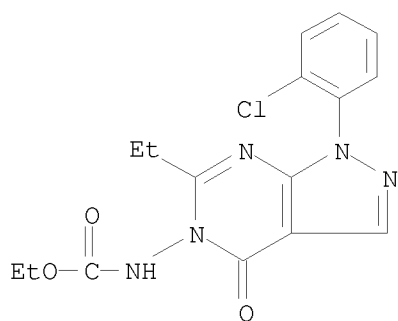
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-amino-1-(2-chlorophenyl)-6-ethyl-1,5-dihydro- (CA INDEX NAME)



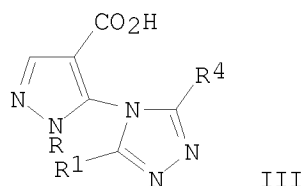
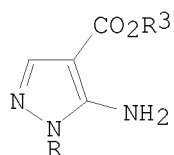
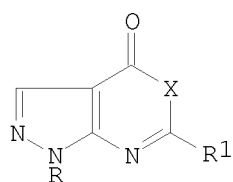
RN 64257-17-6 CAPLUS  
 CN Carbamic acid, (6-ethyl-1,4-dihydro-4-oxo-1-phenyl-5H-pyrazolo[3,4-d]pyrimidin-5-yl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 64257-19-8 CAPLUS  
 CN Carbamic acid, [1-(2-chlorophenyl)-6-ethyl-1,4-dihydro-4-oxo-5H-pyrazolo[3,4-d]pyrimidin-5-yl]-, ethyl ester (9CI) (CA INDEX NAME)



GI



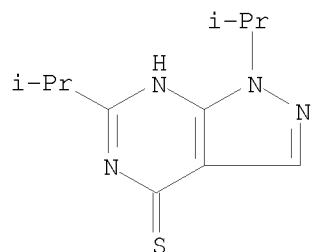
AB    Pyrazolopyrimidines I (R = Ph, 2-ClC<sub>6</sub>H<sub>4</sub>; R<sub>1</sub> = Me, Et; X = NR<sub>2</sub>, R<sub>2</sub> = morpholinoethyl, morpholinopropyl, NH<sub>2</sub>, NHPH) were prepared by condensing EtOCH:C(CN)CO<sub>2</sub>Et with RNHNH<sub>2</sub>, hydrolyzing II (R<sub>3</sub> = Et), cyclizing II (R<sub>3</sub> = H) with (R<sub>1</sub>CO)<sub>2</sub>O, and treating I (X = O), with R<sub>2</sub>NH<sub>2</sub>. Reaction of I (X = O) with H<sub>2</sub>NNHCO<sub>2</sub>Et gave I (X = NNHCO<sub>2</sub>Et), whereas R<sub>4</sub>CONHNH<sub>2</sub> (R<sub>4</sub> = CHMe<sub>2</sub>, CH<sub>2</sub>CN, 2-furyl, 3-pyridyl, 1-naphthyl, 2-naphthyl, 3-indolyl, 2-indolyl, Me, Ph, PhCH<sub>2</sub>) gave III and 1-naphthylacetylhydrazine gave a mixture of I (X = NNHCOCH<sub>2</sub>C<sub>10</sub>H<sub>7</sub>) and III (R<sub>4</sub> = 1-naphthylmethyl).



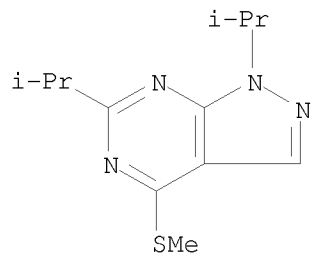
ACCESSION NUMBER: 1966:84620 CAPLUS  
 DOCUMENT NUMBER: 64:84620  
 ORIGINAL REFERENCE NO.: 64:15897g-h,15898a  
 TITLE: 4-Mercaptopyrazolo[3,4-d]pyrimidines  
 INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max  
 PATENT ASSIGNEE(S): CIBA Ltd.  
 SOURCE: 6 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 396924		19660131	CH 1960-1273264	19600511
PRIORITY APPLN. INFO.:			CH	19600511

IT 5494-41-7P, 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol, 1,6-diisopropyl-  
 5494-45-1P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-  
 (methylthio)- 5494-82-6P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,  
 1,6-diisopropyl- 5546-24-7P, 1H-Pyrazolo[3,4-d]pyrimidine,  
 1,6-diisopropyl-4-[(2-piperidinoethyl)thio]- 6109-79-1P,  
 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[3-(diethylamino)propyl]thio]-1,6-  
 diisopropyl-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 5494-41-7 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol, 1,6-diisopropyl- (7CI, 8CI) (CA  
 INDEX NAME)

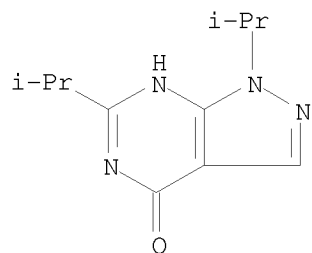


RN 5494-45-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-(methylthio)- (7CI, 8CI)  
 (CA INDEX NAME)



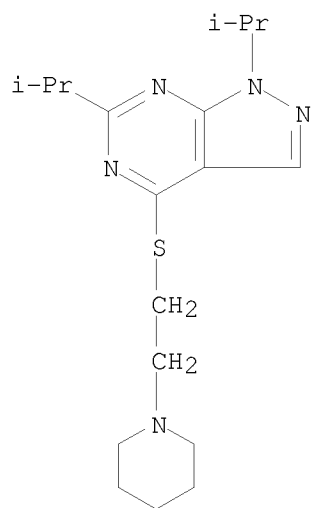
RN 5494-82-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1,6-diisopropyl- (7CI, 8CI) (CA INDEX NAME)



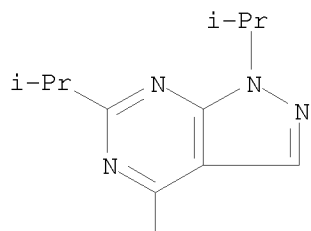
RN 5546-24-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-[(2-piperidinoethyl)thio]- (7CI, 8CI) (CA INDEX NAME)



RN 6109-79-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[3-(diethylamino)propyl]thio]-1,6-diisopropyl- (7CI, 8CI) (CA INDEX NAME)



Et<sub>2</sub>N- (CH<sub>2</sub>)<sub>3</sub>-S

GI For diagram(s), see printed CA Issue.

AB cf. preceding abstract The preparation of I from the corresponding 4-SH compds.

is described. Thus, to a solution of 18.2 g. 1-isopropyl-4-hydroxy-6-methylpyrazolo[3,4-d]pyrimidine, m. 195-6°, in 200 ml. pyridine is added 30 g. P2S5, the mixture refluxed 8 hrs., poured onto 3 l. ice-H2O, and kept overnight to precipitate I (R = H, R1 = Me). Similarly are prepared the

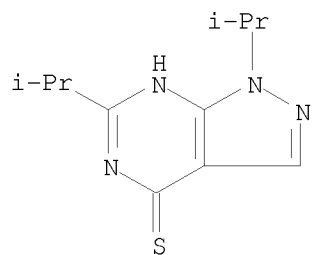
SH

comps. described in the preceding abstract To a solution of 20.8 g. I (R = H, R1 = Me) in 130 ml. 2N NaOH is added 24 ml. Me2SO4 and the mixture stirred at room temperature 1 hr. and kept overnight to precipitate I (R = R1 = Me), m. 66-7° (petroleum ether). Similarly are obtained the SR comps. described in the preceding abstract I possess coronary dilating properties.

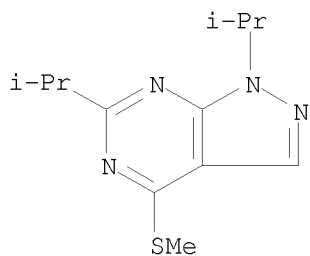
ACCESSION NUMBER: 1966:84619 CAPLUS  
 DOCUMENT NUMBER: 64:84619  
 ORIGINAL REFERENCE NO.: 64:15897d-g  
 TITLE: 4-Mercaptopyrazolo[3,4-d]pyrimidines  
 INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max  
 PATENT ASSIGNEE(S): CIBA Ltd.  
 SOURCE: 4 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 396923		19660131	CH 1960-1273164	19600511
PRIORITY APPLN. INFO.:			CH	19600511

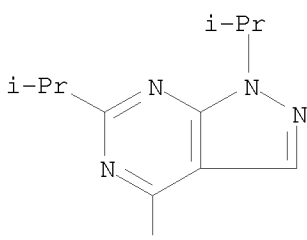
IT 5494-41-7P, 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol, 1,6-diisopropyl-  
 5494-45-1P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-  
 (methylthio)- 5494-46-2P, 1H-Pyrazolo[3,4-d]pyrimidine,  
 4-[[2-(diethylamino)ethyl]thio]-1,6-diisopropyl- 5494-47-3P,  
 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[2-(dimethylamino)ethyl]thio]-1,6-  
 diisopropyl-, hydrochloride 5494-81-5P, 1H-Pyrazolo[3,4-  
 d]pyrimidine, 4-[[2-(dimethylamino)ethyl]thio]-1,6-diisopropyl-  
 5546-20-3P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-[(2-  
 piperidinoethyl)thio]-, hydrochloride 5546-24-7P,  
 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-[(2-piperidinoethyl)thio]-  
 6109-79-1P, 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[3-  
 (diethylamino)propyl]thio]-1,6-diisopropyl-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 5494-41-7 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol, 1,6-diisopropyl- (7CI, 8CI) (CA  
 INDEX NAME)



RN 5494-45-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-(methylthio)- (7CI, 8CI)  
 (CA INDEX NAME)

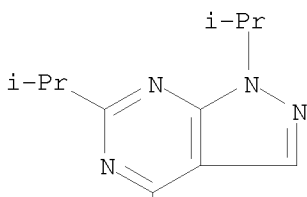


RN 5494-46-2 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[2-(diethylamino)ethyl]thio]-1,6-diisopropyl- (7CI, 8CI) (CA INDEX NAME)



Et<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-S

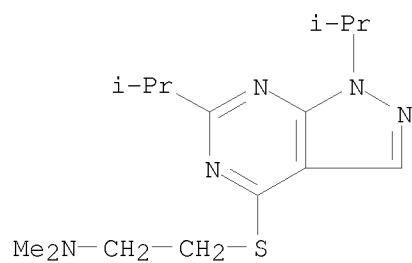
RN 5494-47-3 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[2-(dimethylamino)ethyl]thio]-1,6-diisopropyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



Me<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-S

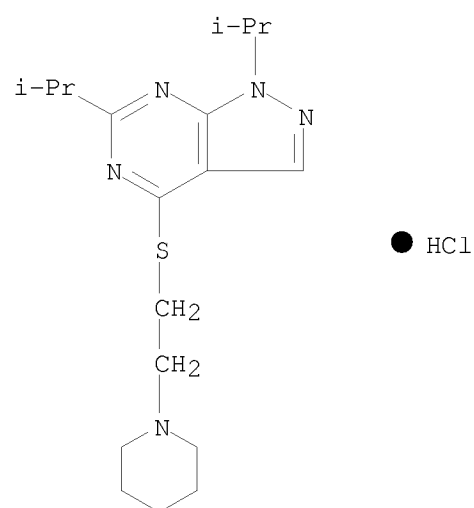
● HCl

RN 5494-81-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[2-(dimethylamino)ethyl]thio]-1,6-diisopropyl- (7CI, 8CI) (CA INDEX NAME)



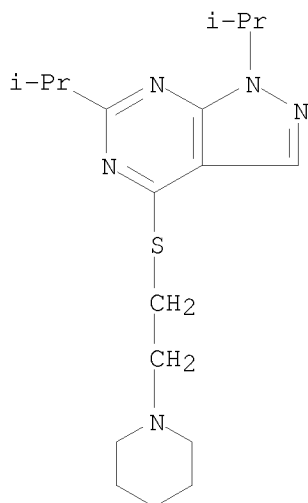
RN 5546-20-3 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-[(2-piperidinoethyl)thio]-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

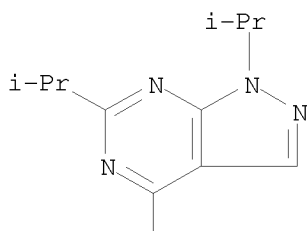


RN 5546-24-7 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-[(2-piperidinoethyl)thio]- (7CI, 8CI) (CA INDEX NAME)



RN 6109-79-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[3-(diethylamino)propyl]thio]-1,6-diisopropyl- (7CI, 8CI) (CA INDEX NAME)



Et<sub>2</sub>N-(CH<sub>2</sub>)<sub>3</sub>-S

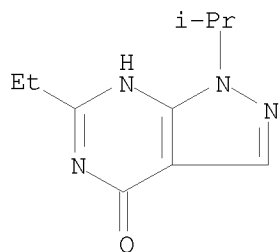
GI For diagram(s), see printed CA Issue.  
 AB cf. following abstract The title compds. (I) are prepared by treating the corresponding 4-halo compds. with thiourea, metal salts of H<sub>2</sub>S, lower-alkyl, amino- or ammonium-lower alkyl mercaptans. Thus, a stirred mixture of 50 ml. PhCH<sub>2</sub>CN, 2.3 g. Na (small pieces), and 9.9 g. 2-isopropyl-3-amino-4-carbethoxypyrazole is heated at 110-20° 4 hrs., cooled, 100 ml. alc. added, the mixture taken to dryness in vacuo, the residue taken up in 150 ml. 2N NaOH, and the alkaline solution washed with CHCl<sub>3</sub> and acidified to pH 5-6 with 6N HCl to precipitate 1-isopropyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (II), m. 165-6° (alc.). A mixture of 10 g. II and 100 ml. POCl<sub>3</sub> is heated at 110° 5 hrs. and evaporated to dryness in vacuo, the residue taken up in H<sub>2</sub>O and extracted with CHCl<sub>3</sub>, the extract washed with N NaOH, dried over Na<sub>2</sub>SO<sub>4</sub>, and the CHCl<sub>3</sub> evaporated in vacuo to yield the 4-Cl (III) analog of II. A solution of III and 8.5 g. thiourea in 150 ml. alc. is refluxed 12 hrs., concentrated to 60 ml., and cooled to afford I (R = H, R<sub>1</sub> = PhCH<sub>2</sub>, m. 145-7°. Similarly are prepared the following I (R, R<sub>1</sub>, b.p. (mm.), and m.p. given): H, Me, --, 226-8°; H, CHMe<sub>2</sub>, --, 170-1°; Me, Me, --, 66-7°; (CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub>, PhCH<sub>2</sub>, --, --(hydrochloride m. 160°); Me, PhCH<sub>2</sub>, --, 84-5°; Me, CHMe<sub>2</sub>, 106-9° (0.05), --; (CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub>, CHMe<sub>2</sub>, 138-40° (0.05),

--; (CH<sub>2</sub>)<sub>3</sub>NEt<sub>2</sub>, CHMe<sub>2</sub>, 149-51° (0.02), --; 2-(piperidine)ethyl,  
CHMe<sub>2</sub>, --, -- (hydrochloride m. 163-5°); (CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>, CHMe<sub>2</sub>, --, --  
(hydrochloride m. 178-80°).



ACCESSION NUMBER: 1966:84617 CAPLUS  
 DOCUMENT NUMBER: 64:84617  
 ORIGINAL REFERENCE NO.: 64:15896h,15897a-b  
 TITLE: Novel pyrazolopyrimidines  
 INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max  
 PATENT ASSIGNEE(S): CIBA Ltd.  
 SOURCE: 3 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

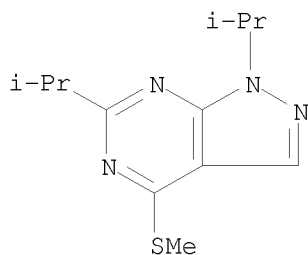
	PATENT NO. -----	KIND ----	DATE -----	APPLICATION NO. -----	DATE -----
	CH 396927		19660113	CH 1960-509965	19600511
PRIORITY APPLN. INFO.:				CH	19600511
IT	5543-55-5P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-ethyl-1-isopropyl-				
	RL: PREP (Preparation)				
	(preparation of)				
RN	5543-55-5 CAPLUS				
CN	1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-ethyl-1-isopropyl- (7CI, 8CI) (CA INDEX NAME)				



AB The title compds. are prepared by cyclization of substituted pyrroles. Thus, a mixture of 30 g. 2-isopropyl-3-amino-4-cyanopyrazole (I) and 68 ml. Ac<sub>2</sub>O is refluxed 10 hrs., the mixture evaporated to dryness, the residue recrystd. from Et<sub>2</sub>O and subsequently from H<sub>2</sub>O, and the mother liquor concentrated to give a viscous mass (II) containing the acetylamino derivative of I. A mixture of II (3.84 g.), 14 ml. 10% aqueous KOH, and 30 ml. 3% H<sub>2</sub>O<sub>2</sub> is heated on a steam bath 0.5 hr., filtered, and the filtrate acidified with 2N HCl to give 1-isopropyl-4-hydroxy-6-methylpyrazolo[3,4-d]pyrimidine (III), m. 195-6° (alc.). Similarly prepared is the 6-Et derivative of III, m. 180-2° (EtOH). The compds. possess coronary dilating properties.

L7 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

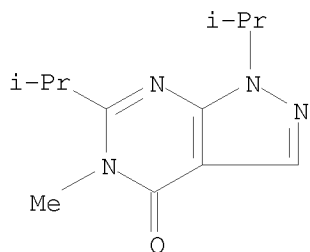
ACCESSION NUMBER: 1966:79294 CAPLUS  
DOCUMENT NUMBER: 64:79294  
ORIGINAL REFERENCE NO.: 64:14897f-g  
TITLE: Relation between synergism and metabolism of  
dimethoate in mammals and insects  
AUTHOR(S): Uchida, T.; Zschintzsch, J.; O'Brien, R. D.  
CORPORATE SOURCE: Cornell Univ., Ithaca, NY, USA  
SOURCE: Toxicology and Applied Pharmacology (1966), 8(2),  
259-265  
CODEN: TXAPA9; ISSN: 0041-008X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
IT 5494-45-1P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-  
(methylthio)-  
RL: PREP (Preparation)  
(preparation of)  
RN 5494-45-1 CAPLUS  
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-(methylthio)- (7CI, 8CI)  
(CA INDEX NAME)



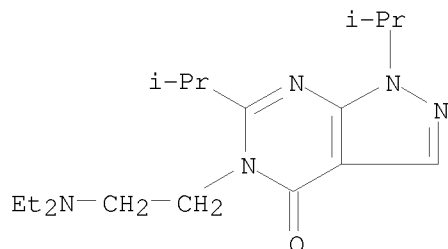
AB Toxicol. Appl. Pharmacol. 8(2), 259-65(1966)(Eng). EPN (Et p-nitrophenyl thiono-benzenephosphate) synergizes the toxicity of dimethoate profoundly in female mice, mildly in female guinea pigs, and not at all in female houseflies (Wilson and G strains) or milkweed bugs. These findings parallel the observations that EPN blocks di-methoate metabolism profoundly (80%) in mice, less in guinea pigs (60%), and not at all in houseflies and milkweed bugs. Synergism in this pair of compds. is caused by blockade of metabolism. However, the ability of EPN to distinguish between the amidase and phosphatase pathways is not so clear-cut as in the corresponding carboxyesterase and phosphatase pathways for malathion, whose toxicity is also synergized by EPN.

ACCESSION NUMBER: 1965:22609 CAPLUS  
 DOCUMENT NUMBER: 62:22609  
 ORIGINAL REFERENCE NO.: 62:4037c-e  
 TITLE: Pyrazolo[3,4-d]pyrimidines  
 PATENT ASSIGNEE(S): CIBA Ltd.  
 SOURCE: 7 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 973361		19641028	GB 1961-17103	19610510
PRIORITY APPLN. INFO.:			CH	19600511
IT 1143-77-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,6-diisopropyl-5-methyl- 1237-01-0P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro- 1,6-diisopropyl- RL: PREP (Preparation) (preparation of) RN 1143-77-7 CAPLUS CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,6-diisopropyl-5-methyl- (7CI, 8CI) (CA INDEX NAME)				



RN 1237-01-0 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-  
 1,6-diisopropyl- (7CI, 8CI) (CA INDEX NAME)

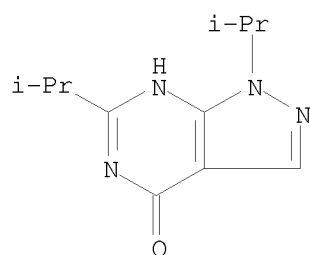


GI For diagram(s), see printed CA Issue.  
 AB The title compds. (I) were prepared by alkylating a 1,6-disubstituted 4-hydroxypyrazolo[3,4-d]pyrimidine with a dialkylaminoalkyl chloride or Me<sub>2</sub>SO<sub>4</sub>. Thus, a solution of 1.15 g. Na in 40 ml. EtOH was added to 14.1 g. 1-sec-butyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine followed by 7.5 g.

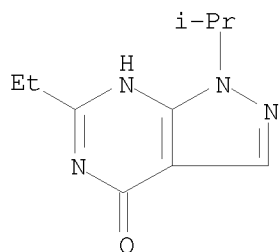
Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl and the mixture refluxed 4 hrs. to give the hydrochloride of I (R<sub>1</sub> = sec-Bu, R<sub>2</sub> = Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, R<sub>3</sub> = PhCH<sub>2</sub>), m. 147-8°. The following I were prepared similarly (R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, m.p. free base, and m.p. hydrochloride given): iso-Pr, Me, PhCH<sub>2</sub>, 96-7°, --; iso-Pr, Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, PhCH<sub>2</sub>, 115-17°, 229-31°; iso-Pr, Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, PhCH<sub>2</sub>, --, 202-3°; iso-Pr, Et<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>, PhCH<sub>2</sub>, 70-1°, 173-5°; Me, Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, PhCH<sub>2</sub>, 83-5°, 219°; Ph, Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, PhCH<sub>2</sub>, 103-5°, 225°; iso-Pr, Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, Me, --, --; iso-Pr, Me, iso-Pr, 75-7°, --; iso-Pr, Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, iso-Pr, --(b0.05 138-40°), --; iso-Pr, Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, Ph<sub>2</sub>CH, 124-5°, --. The title compds. had coronary dilating properties.

ACCESSION NUMBER: 1964:68272 CAPLUS  
 DOCUMENT NUMBER: 60:68272  
 ORIGINAL REFERENCE NO.: 60:12027a-c  
 TITLE: 1-Isopropyl-4-hydroxypyrazolo[3,4-d]pyrimidines  
 INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max  
 PATENT ASSIGNEE(S): CIBA Ltd.  
 SOURCE: 4 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

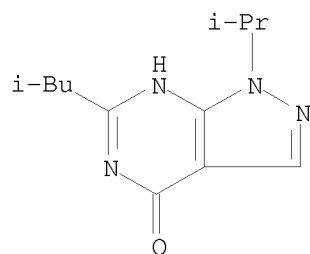
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1156415		19631031	DE	
CH 396926			CH	
PRIORITY APPLN. INFO.:			CH	19600511
IT 5494-82-6P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1,6-diisopropyl-				
5543-55-5P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-ethyl-1-isopropyl-				
88618-14-8P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,				
6-isobutyl-1-isopropyl-				
RL: PREP (Preparation)				
(preparation of)				
RN	5494-82-6 CAPLUS			
CN	1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1,6-diisopropyl- (7CI, 8CI) (CA INDEX NAME)			



RN 5543-55-5 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-ethyl-1-isopropyl- (7CI, 8CI) (CA INDEX NAME)



RN 88618-14-8 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-isobutyl-1-isopropyl- (7CI) (CA INDEX NAME)

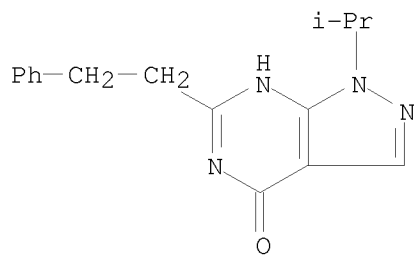


GI For diagram(s), see printed CA Issue.

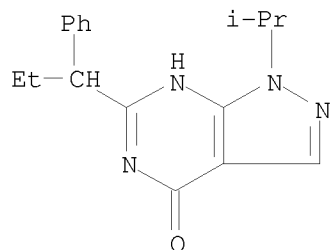
AB 2-Isopropyl-3-amino-4-carbethoxypyrazole (39.6 g.) in 160 cc. isobutyronitrile and 9.2 g. Na was heated slowly over 1 hr. to 110°, and the mixture kept 4 hrs. at 110° to give 16 g. I (R = iso-Pr), m. 175-7°. Similarly prepared were the following I (R and m.p. given): Me, 195-6°; Me<sub>2</sub>CHCH<sub>2</sub>, 114-16°; Et, 180-2°. I are coronary dilators.

ACCESSION NUMBER: 1964:16883 CAPLUS  
 DOCUMENT NUMBER: 60:16883  
 ORIGINAL REFERENCE NO.: 60:2981a-e  
 TITLE: 4-Hydroxypyrazolo[3,4-d]pyrimidines  
 INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max  
 PATENT ASSIGNEE(S): CIBA Ltd.  
 SOURCE: 10 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	DE 1153023		19630822	DE	
	CH 396925			CH	
	GB 937724			GB	
PRIORITY APPLN. INFO.:				CH	19600511
IT	93022-45-8P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1-isopropyl-6-phenethyl- 93726-17-1P, 1H-Pyrazolo[3,4- d]pyrimidin-4-ol, 6-( $\alpha$ -ethylbenzyl)-1-isopropyl- RL: PREP (Preparation) (preparation of)				
RN	93022-45-8 CAPLUS				
CN	1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1-isopropyl-6-phenethyl- (7CI) (CA INDEX NAME)				



RN 93726-17-1 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-( $\alpha$ -ethylbenzyl)-1-isopropyl-  
 (7CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.  
 AB 1-R1, 3-R2, 6-R3-substituted 4-hydroxy pyrazolo[3,4-d]pyrimidines (R1 = H,  
 alkyl, hydroxyalkyl, or oxaalkyl; R2 = H or low-mol.-weight alkyl; R3 =

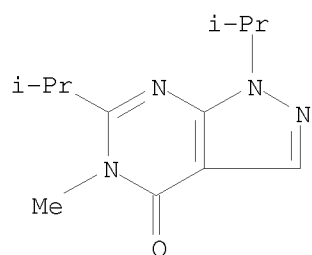
eventually substituted phenylalkyl or diphenylalkyl radicals) are prepared. Thus, 19.7 g. 2-isopropyl-3-amino-4-carbethoxypyrazole and 45 g.  $\beta$ -phenylpropionitrile in 30 cc. absolute PhMe are added to 4.6 g. powdered Na in 85 cc. absolute PhMe at 90-5° with stirring, the mixture stirred 5 hrs. at 90-5°, 50 cc. alc. added, the solution evaporated to dryness, the residue extracted with N NaOH and PhMe, and the alkaline solution neutralized with 6N HCl to precipitate 8.7 g. 1-isopropyl-4-hydroxy-(6-R-substituted)-pyrazolo[3,4-d]pyrimidine(I) (R =  $\beta$ -phenylethyl), m. 124-5° (alc.). Similarly prepared are the following I (R and m.p. given): m-hydroxybenzyl, 226-7° (alc.); p-chlorobenzyl (II), 181-2° (alc.); 3,4,5-trimethoxy-phenylmethyl, 195-6° (alc.); p-ethoxybenzyl, 175-6° (alc.); m-methoxybenzyl, 155-8° (alc.); o-methoxybenzyl, 157-9° (EtOH); 2-methyl-3-methoxybenzyl, 150-1° (EtOH); diphenylmethyl, 226-7° (EtOH);  $\alpha$ -phenylpropyl, 142-3° (alc.). Also prepared are the following 1-methyl-4-hydroxy-(6-R-substituted)-pyrazolo[3,4-d]pyrimidines (R and m.p. given): benzyl, 236-7° (EtOH); 3,4,5-trimethoxyphenylmethyl, 245° (CHCl<sub>3</sub>-petr. ether); p-chlorobenzyl, 268-70° (HCONMe<sub>2</sub>-H<sub>2</sub>O); 2,3-dimethoxyphenylmethyl, 190-1° (alc.). The following (1-R-substituted)-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidines are prepared (R and m.p. given): sec-butyl, 154-5° (alc.); pent-3-yl, 144-5° (absolute alc.);  $\beta$ -hydroxyethyl, 194-5° (alc.); 1-ethoxybut-3-yl, 111-12° (MeOH-H<sub>2</sub>O); H, 290-2° (EtOH); 3-methylbut-2-yl, 157-8° (EtOH). Also prepared are these starting materials: 2-( $\beta$ -hydroxyethyl)-3-amino-4-carbethoxypyrazole, b0.6 180°, m. 89-91°; 2-[1-ethoxybut-3-yl]-3-amino-4-carbethoxypyrazole, b0.1 120-5°; 2-isopropyl-3-[ $\alpha$ -ethoxy- $\beta$ -(p-chlorophenyl)ethylidenamino]pyrazole-4-carboxamide; 2-isopropyl-3-(p-chlorophenylacetamido)-4-carboxypyrazole; 1-isopropyl-4-oxo-6-(p-chlorobenzyl)pyrazolo[3,4-d]oxazine; 2-isopropyl-3-(p-chlorophenylacetamido)-4-pyrazolecarbonitrile.



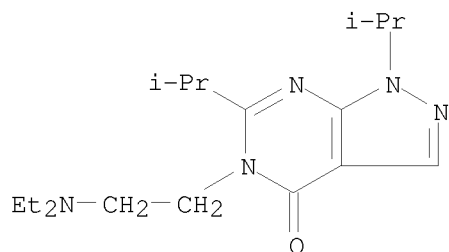
ACCESSION NUMBER: 1963:469189 CAPLUS  
 DOCUMENT NUMBER: 59:69189  
 ORIGINAL REFERENCE NO.: 59:12820a-h,12821a  
 TITLE: Pyrazolo[3,4-d]pyrimidines  
 INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max  
 PATENT ASSIGNEE(S): CIBA Ltd.  
 SOURCE: 7 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1149013		19630522	DE	
			CH	19600511

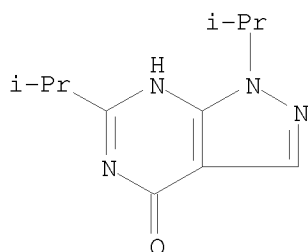
PRIORITY APPLN. INFO.:  
 IT 1143-77-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,  
 1,5-dihydro-1,6-diisopropyl-5-methyl- 1237-01-0P,  
 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-  
 1,6-diisopropyl- 5494-82-6P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,  
 1,6-diisopropyl-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 1143-77-7 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,6-diisopropyl-5-methyl-  
 (7CI, 8CI) (CA INDEX NAME)



RN 1237-01-0 CAPLUS  
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-  
 1,6-diisopropyl- (7CI, 8CI) (CA INDEX NAME)



RN 5494-82-6 CAPLUS  
 CN 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1,6-diisopropyl- (7CI, 8CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB 4-Oxo-4,5-dihydropyrazolo[3,4-d]pyrimidines (I), possessing vasodilating ability, are described in which R1 = H, alkyl or phenyl group, R2 = H or lower alkyl group, R3 = HO, halogen, NR5R6 (R5 and R6 = H, alkyl groups or joined together through O, S, or N) (or the position may be unsubstituted), R4 = alkyl or aralkyl group. The most active compds., I (R1 = iso-Pr, R2 = H, R3 = Et2NCH2CH2, R4 = PhCH2) (II) and I (R1 = sec-Bu, R2 = H, R3 = Et2NCH2CH2, R4 = PhCH2) (III) at a concentration of 10  $\gamma$ /ml. increase coronary blood flow 78-73% in the Langendorf isolated dog heart procedure. In the same test, 1-isopropyl-4-diethylaminopyrazolo-[3,4-d]pyrimidine (CA 55, 13457a) at the same concentration causes an increase

of

60%. In the compds. described below R2 = H. Na (2.3 g.) is finely dispersed in 50 ml. PhCH2CN and 9.9 g. 2-isopropyl-3-amino-4-carbethoxypyrazole (IV) added. The mixture is heated to 110-20° with stirring for 4 hrs. and cooled, 100 ml. alc. is added, and the mixture evaporated to dryness in vacuo. The residue is taken into 150 ml. 2N NaOH, extracted with CHCl3 to remove undissolved material and adjusted to pH 5 to 6 with 6N HCl to yield 1-isopropyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (V), m. 165-6° (alc.). V in 30 ml. N NaOH treated with Me2SO4 gave I (R1 = iso-Pr, R3 = Me, R4 = PhCH2) (VI), m. 96-7°. The procedure similar to that used for the preparation of IV is used to prepare 1-sec-butyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (VII), m. 154-5°. A solution of 1.15 g. Na in 40 ml. absolute alc. is added to 14.4 g. VII in 60 ml. absolute alc. and refluxed 4 hrs. after the addition of 7.5 g. Et2NCH2CH2Cl to give after HCl treatment 15.4 g. III.HCl, m. 147-8°. Similarly, 13.4 g. V is allowed to react with 1.2 g. Na in 300 ml. absolute EtOH, then with 5.5 g. Me2NCH2CH2Cl to yield 10.2 g. I (R1 = iso-Pr, R3 = Me2NCH2CH2, R4 = PhCH2) (VIII), m. 115-17°; VIII.HCl m. 229-31°. V, as the Na salt, is allowed to react with Et2NCH2CH2Cl to yield I (R1 = iso-Pr, R3 = Et2NCH2CH2, R4 = PhCH2).HCl, m. 202-3°. When V, as the Na salt, is allowed to react with Et2NCH2CH2CHCl, II.HCl, m. 173-5°, is isolated. 1-Methyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (IX) is prepared from 2-methyl-3-amino-4-carbethoxypyrazole and PhCH2CN (X) by the procedure for the preparation of V. The reaction of 12 g. IX with 1.2 g. Na in 25 ml.

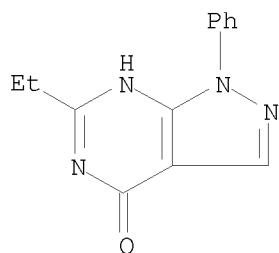
absolute

alc. followed by the addition of 6 g. Et2NCH2CH2Cl leads to the isolation of I (R1 = Me, R3 = Et2NCH2CH2, R4 = PhCH2) (XI), m. 83-5° XI.HCl m. 219°. Likewise, 2-phenyl-3-amino-4-carbethoxypyrazole and X yields 1-phenyl-6-benzyl-4-hydroxypyrazolo[3,4-d]pyrimidine, m. 264-5° which is allowed to react as the Na salt with Et2NCH2CH2Cl to give I (R1 = Ph, R3 = Et2NCH2CH2, R4 = PhCH2) (XII), m. 103 5° XII.HCl m. 225°. To an ice-cooled solution of 9.9 g. IV in 50 ml. MeCN is added 2.3 g. Na and the temperature of reaction kept below 30°. After the addition, the mixture is heated to 90-95° for 4 hrs., cooled, and 100

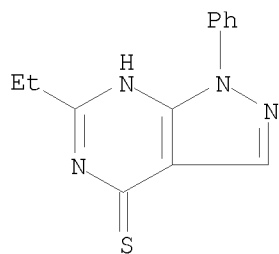
ml. EtOH added. The mixture is evaporated to dryness and residue treated with 150 ml. 2N NaOH, extracted with CHCl<sub>3</sub> and the aqueous layer adjusted to pH 3 to 4 with 5N HCl and the precipitate crystallized from alc. to give 1-isopropyl-4-hydroxy-6-methylpyrazolo[3,4-d]pyrimidine (XIII), m. 195-6°. The reaction of 9.1 g. XII with 1.2 g. Na in 150 ml. absolute alc., followed by the addition of 7 g. Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl, and 4 hrs. reflux yields 7 g. I (R<sub>1</sub> = iso-Pr, R<sub>3</sub> = Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, R<sub>4</sub> = Me), m. 166-8°. 1,6-Diisopropyl-4-hydroxypyrazolo[3,4-d]pyrimidine (XIV), m. 175-7°, is prepared from iso-BuCN and IV in the presence of Na. A solution of 11 g. XIV in 75 ml. 2N NaOH solution is stirred at room temperature with 6.3 g. Me<sub>2</sub>SO<sub>4</sub> and allowed to stand overnight to yield 9 g. I (R<sub>1</sub> = R<sub>4</sub> = iso-Pr, R<sub>3</sub> = Me), m. 175-7°. XIV (10 g.) is added to a solution of 1.05 g. Na in 150 ml. absolute alc., stirred 1 hr. at room temperature and 6.5 g. Et<sub>2</sub>. NCH<sub>2</sub>CH<sub>2</sub>Cl is added. The mixture is refluxed 4 hrs., evaporated to dryness in vacuo and the residue dissolved in 100 ml. N HCl, adjusted to a pH with NaOH solution and the oil that results is extracted with Et<sub>2</sub>O. The residue, after removal of the Et<sub>2</sub>O, is distilled to yield 9 g. I (R<sub>1</sub> = R<sub>4</sub> = iso-Pr, R<sub>3</sub> = Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>), b<sub>0.05</sub> 138-40°. A mixture of 20 g. X and 19.7 g. IV is warmed to 70° and 2.3 g. of Na in small pieces added. The mixture is heated 4 hrs. at 110-20°, allowed to cool, and the excess Na destroyed by the addition of alc. The mixture is evaporated to dryness in vacuo, the residue treated with 300 ml. H<sub>2</sub>O and 2N HCl added to adjust the pH to 3. The precipitate is removed by filtration and crystallized from petr. ether to yield 1-isopropyl-4-hydroxy-6-diphenylmethylpyrazolo[3,4-d]pyrimidine (XV), m. 226 7°. XV(5.2 g.) is added to a solution of 0.35g. Na in 150 ml. EtOH, the mixture stirred at room temperature and 2.1 g. Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>Cl is added. The mixture is refluxed 4 hrs. and evaporated to dryness in vacuo and the residue crystallized from petr. ether to yield 3.8 g. I (R<sub>1</sub> = iso-Pr, R<sub>3</sub> = Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, R<sub>4</sub> = Ph<sub>2</sub>CH), m. 124-5°.

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 NAME)



GI For diagram(s), see printed CA Issue.  
 AB cf. C.A. 52, 13741h. A synthesis of 6-alkyl-4-hydroxypyrazolo  
 [3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:COH (I) was devised from the  
 corresponding 5-acylamino-4-cyanopyrazoles, R3CONHC:C(CN).CR2.N.NR1 (II)  
 which were in turn prepared from 5-amino-4-cyanopyrazoles,  
 R1N.N:CH.C(CN):CNH2 (III). Evidence was presented to show that the  
 5-acylaminopyrazole-4-carboxamide is an intermediate in this cyclization.  
 Chlorination of I yielded the corresponding 6-alkyl-4-chloropyrazolo  
 [3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:CCl (IV). Nucleophilic  
 displacement of the Cl in IV resulted in the preparation of a large number of

6-alkylpyrazolo[3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:CNR4R5 (V). III (R1 = 3-Me) (80 g.) and 250 ml. Ac2O refluxed 10 hrs., excess Ac2O distilled in vacuo, the sirupy substance poured into 30 ml. C6H6, stirred several min., and crystallized gave 89 g. II (R1 = R2 = H, R3 = Me), crystals from H2O. Similarly II (R1 = R3 = Me, R2 = H) was prepared and the product recrystd. from H2O to a white powder. III (R1 = Ph) (150 g.) treated 19 hrs. under reflux with 200 ml. Ac2O, excess solvent removed, the residue treated with a small amount of C6H6, and Skellysolve (b. 60°), and the product isolated gave 171 g. II (R1 = Ph, R2 = H, R3 = Me) crystallized from H2O. The following II were thus prepared (R1, R2, R3, m.p., % yield, and recrystn. solvent given): H, H, Me, 221-2°, 76, H2O; Me, H, Me, 210-11°, 72, H2O; Ph, H, Me, 155-6°, 92, H2O; o-ClC6H4, H, Me, 175-5.5°, 82, alc., H2O; p-ClC6H4, H, Me, 173-5°, 96, alc, H2O; p-BrC6H4, H, Me, 175-5° (sic), 98, alc., H2O; p-O2NC6H4, H, Me, 198-200°, 95, alc., H2O; p-MeC6H4, H, Me, 128°, 96, alc., H2O; AcOCH2CH2, H, Me, 155-7°, 81, alc. II (R1 = Ph, R2 = H, R3 = Me) (30 g.) added at 15-20° to 120 ml. concentrated H2SO4, the clear solution stirred 0.5 hr., then poured onto 1 kg.

ice,

neutralized with concentrated NH4OH, the solid collected, washed, dried, and recrystd. from C6H6 and MeOH gave 20 g. 5-amino-1-phenylpyrazole-4-carboxamide (VI), m. 172-5°, identical with the product obtained from the hydrolysis of 5-amino-4-cyano-1-phenylpyrazole. VI (20 g.) and 200 ml. Ac2O refluxed 15 hrs., and purification gave 15 g. 6-methyl-4-oxo-1-phenylpyrazolo [3,4-d]-5,7-oxazine (VII), m. 184.5-5.5° (sublimed at 145°) (C6H6-C7H16). VII (2.5 g.) kept 2 hrs. at room temperature with 200 ml. H2O and 2 g. KOH, heated 10 hrs., acidified, and the precipitate collected gave 2 g.

5-acetamido-1-phenylpyrazole-4-

carboxylic acid (VIII), m. 201-2° (AcOH), readily lost CO2 on heating. The 5-acetylamido group was retained in warm alkaline solution but hydrolyzed readily in cold acidic medium. VII (2 g.) left 0.5 hr. at room temperature with 100 ml. alc. NH3, heated briefly until a solid product

precipitated,

and the product collected gave 5-acetamido-1-phenylpyrazole-4-carboxamide (IX), m. 301-2°, relatively unstable. The m.p. of IX was the same as that for I (R1 = Ph, R2 = Me) and was undepressed in mixed m.p. The ultraviolet absorptions for IX at 230 mμ and for I at 233 and 269 mμ, were different. Thus IX cyclized at elevated temps. during the m.p. determination I were prepared by the following method. II (R1 = R2 = H,

R3 =

Me) (1.5 g.); 7 ml. 10% KOH, and 15 ml. 3% H2O2 warmed 0.5 hr. at 70-5°, the mixture acidified, the solid collected, and repptd. with dilute KOH and AcOH gave 1.1 g. I (R1 = H, R2 = Me). II (R1 = R3 = Me, R2 = H) (121 g.) warmed 10 hrs. at 70° with 1500 ml. 3% H2O2 and 400 ml. 10% KOH gave 103 g. I (R1 = R2 = Me), needles, sublimed at 180°. II (R1 = Ph, R2 = H, R3 = Me) (14.5 g.) in 5 g. KOH and 200 ml. 3% H2O2 warmed 5 hrs. at 70-5° and acidified gave 14 g. crude I (R1 = Ph, R2 = Me), m. 298-300°. IX(1 g.) heated 20 min. at 70° with 100 ml. 10% KOH, then acidified, the solid collected and recrystd. gave 0.8 g. product identical with that from the preceding experiment I (R1 = R2 = Me) (25 g.) and 400 ml. POCl3 refluxed 2 hrs., excess solvent removed, the sirup poured onto 1 kg. ice, the suspension left 15 min., extracted with CHCl3, dried, solvent removed at room temperature, and the solid isolated gave 24 g. IV (R1 = R2 = Me) as needles. I (R1 = H, R2 = Me) (50 g.) refluxed 2 hrs. with 140 ml. PhNMe2 and 1 l. POCl3, excess POCl3 removed, the residue poured on ice, and extracted with Et2O gave 35 g. IV (R1 = H, R2 = Me), unstable. I (R1 = p-O2NC6H4, R2 = Me) (20 g.) refluxed 3 hrs. with 250 ml. POCl3 gave 17.5 g. IV (R1 = p-O2NC6H4, R2 = Me) as a yellow powder.

Preparation of 1-alkyl(aryl)-6-alkyl-4-mercaptopyrazolo[3,4-d]pyrimidines X) (R1 = 1-substituent, R2 = 6-substituent) was achieved by the following two methods: (method 1) I (R1 = Ph, R2 = Me) (11 g.) and 50 g. P2S6 added portionwise during 45 min. to 400 ml. Tetralin (preheated to 165°), the temperature allowed to rise to 185°, then heated 6 hrs. to 190-5°, the solution cooled overnight, filtered, the product dissolved in dilute KOH and precipitated with AcOH gave 5.5 g. X (R1 = Ph, R2 = Me);

method

2) IV (R1 = Ph, R2 = Me) (14 g.) and 14 g. CS(CH2)2 in 120 ml. alc. refluxed 4 hrs., the product collected and washed well with alc. and H2O, and the product purified by precipitation from a hot basic solution with AcOH

gave

11.5 g. X (R1 = Ph, R2 = Me). All the other X were prepared by essentially the same procedure as method 2. 1-Alkyl(aryl)-6-alkyl-4-alkylthiopyrazolo[3,4-d]pyrimidines (XI) (R1 = 1-substituent, R2 = 6-substituent, R3 = S-substituent) were prepared as follows: X (R1 = R2 = Me) (13 g.), 40 ml. 4N KOH, 18 g. MeI, and 30 ml. MeOH shaken 0.5 hr. in a separatory funnel, the contents left overnight at 40°, and the solid collected gave 12.5 g. XI (R1 = R2 = R3 = Me). X (R1 = Ph, R2 = Me) (1 g.) added to 200 ml. H2O containing 15 g. KOH and 21 g. EtI, treated with 100 ml. alc., refluxed 5 hrs., and reduced in volume, until an oily product solidified gave 3 g. XI (R1 = Ph, R2 = Me, R3 = Et). 4-Alkoxy-1-alkyl(aryl)-6-methylpyrazolo[3,4-d]pyrimidines (XII) (R1 = 1-substituent, R2 = O-substituent) were prepared as follows: IV (R1 = p-MeC6H4, R2 = Me) (5.5 g.) and 100 ml. alc. left 2 hrs. at room temperature with 2 g. Na in 70

ml.

alc., heated 40 min. on the steam bath, and NaCl removed, the filtrate treated with 50 ml. H2O, and left overnight in the cold gave 3.1 g. XII (R1 = p-MeC6H4, R2 = Et). Other XII were prepared as above. The following N:CR2.N:CR3.C:C.NR1.N:CH were prepared by the above methods (R1, R2, R3, m.p., % yield, and recrystn. solvent given): H, Me, OH, 336-8°, 73.5, AcOH; H, Me, Cl, 140° (decomposition), 70.0, C6H6; H, Me, SH, above 300°, 80, repptd.; H, Et, OH, above 300°, 82, alc., H2O; Me, Me, OH, 277-8°, 72.5, alc., H2O; Me, Me, Cl, 74°, 70.2, C7H16; Me, Me, OMe, 107.5-8.5°, 67.5, MeOH; Me, Me, SH, 264-5°, 98, repptd.; Me, Me, SMe, 74-5°, 90.2, MeOH, H2O; CH2CH2OH, Me, OH, 265-6°, 54.8, H2O; Ph, Me, Cl, 85-6°, 83.5, C7H16; Ph, Me, SH, 268.5°, 83.3, repptd.; Ph, Me, OMe, 121.5-2.0°, -, MeOH; Ph, Me, OEt, 95-5.5°, -, alc.; Ph, Me, SMe, 135-7°, -, MeOH, H2O; Ph, Me, SEt, 86-8°, -, alc., H2O; Ph, Et, OH, 295°, 88.5, alc., H2O; Ph, Et, SH, 248-9°, 91.6, repptd.; p-MeC6H4, Me, OH, 298-300°, 93.6, alc., H2O; p-MeC6H4, Me, Cl, 89-91°, 78.1, C7H16; p-MeC6H4, Me, OMe, 121-2°, 81.2, MeOH; p-MeC6H4, Me, OEt, 93-4°, 53, alc.; o-ClC6H4, Me, Cl, 121°, 77.8, C6H14; p-BrC6H4, Me, OH, above 315°, 86.6, alc., H2O; p-BrC6H4, Me, Cl, 130.5-31°, 88.7, C6H14; p-ClC6H4, Me, OH, above 310°, 94.5, alc., H2O; p-ClC6H4, Me, Cl, 129°, 82.6, C7H16; p-ClC6H4, Me, SH, above 305°, 75.2, repptd.; p-O2NC6H4, Me, OH, above 310°, 90, repptd.; p-O2NC6H4, Me, Cl, 184°, 82, PhMe. V were prepared by the following methods: (method A) IV (R1 = H, R2 = Me) (10 g.) and 120 ml. alc. NH3 heated 8 hrs. in a bomb at 160°, the product evaporated to dryness, the residue refluxed with dilute HCl, the solution treated with C, filtered, and the product repptd. with NH4OH, filtered, and recrystd. gave 6.5 g. V (R1 = R4 = R5 = H, R2 = Me); (method B) the above IV (5 g.) added to 7 g. BuNH2, and 120 ml. alc. and the mixture refluxed 7 hrs. gave 3 g. V (R1 = R4 = H, R2 = Me, R5 = Bu). IV (R1 = Ph, R2 = Me) (5 g.) refluxed 40 min. with 8 g. p-ClC6H4NH2 and 75 ml. alc. and the mixture filtered after cooling 3 hrs. in an ice bath gave 6.2 g. crude V (R1 = Ph, R2 = Me, R4 = H, R5 = p-ClC6H4). IV (R1 =

p-ClC<sub>6</sub>H<sub>4</sub>, R<sub>2</sub> = Me) (9 g.) refluxed on a steam bath to near dryness with 160 ml. alc. containing 10 g. PhCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> and the residue added to MeOH gave 11 g. V (R<sub>1</sub> = p-ClC<sub>6</sub>H<sub>4</sub>, R<sub>2</sub> = Me, R<sub>4</sub> = H, R<sub>5</sub> = CH<sub>2</sub>CH<sub>2</sub>Ph); (method C) IV (R<sub>1</sub> = R<sub>2</sub> = Me) (5.5 g.), 5.5 g. furfurylamine, and 200 ml. alc. heated 8 hrs. on a steam bath, then evaporated, the residue stirred with 30 ml. 10% KOH, the alkaline solution decanted, the sirup refluxed 2 hrs. with 100 ml. C<sub>6</sub>H<sub>6</sub>, and

the

solution, filtered and evaporated to dryness gave 4 g. V (R<sub>1</sub> = R<sub>2</sub> = Me, R<sub>4</sub> = H, R<sub>5</sub> = furfuryl as white needles. IV (R<sub>1</sub> = Ph, R<sub>2</sub> = Et) (13 g.) in 150 ml. alc. treated slowly with 13 g. PhCH<sub>2</sub>NH<sub>2</sub> in 50 ml. alc., the mixture refluxed 12 hrs., the solvent removed, and the product treated with C<sub>6</sub>H<sub>6</sub> and several drops MeOH, and refrigerated gave 8 g. V (R<sub>1</sub> = Ph, R<sub>2</sub> = Et, R<sub>4</sub> = H, R<sub>5</sub> = CH<sub>2</sub>Ph). The following V were prepared by these methods (R<sub>1</sub>, R<sub>2</sub>, R<sub>4</sub>, R<sub>5</sub>, m.p., method of preparation, % yield, and recrystn. solvents given): H, Me, H, H, above 300°, A, 73, alc., H<sub>2</sub>O; H, Me, H, Me, above 300°, B, 60, alc., H<sub>2</sub>O; H, Me, H, Et, 273-4°, B, 56, alc.; H, Me, H, Pr, 220-2°, B, 49.1, alc.; H, Me, H, CH<sub>2</sub>Ph, 241°, B, 87.2, alc.; H, Me, H, furfuryl, 243-4°, C, 59, alc.; Me, Me, H, H, 251-2°, A, 90, alc., H<sub>2</sub>O; Me, Me, H, Me, 136-8°, B, 77.2, H<sub>2</sub>O; Me, Me, H, Et, 131.5-2.0°, C, 66.9, PhMe, C<sub>7</sub>H<sub>16</sub>; Me, Me, H, CH<sub>2</sub>Ph, 180-2°, B, 83, alc.; Me, Me, H, furfuryl, 140-1.5°, C, 54.6, alc.; Me, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>, 223.5-4.0°, B, 60, alc.; Me, Me, H, p-ClC<sub>6</sub>H<sub>4</sub>, 231.5°, B, 67, alc., H<sub>2</sub>O; Me, Me, H, p-MeC<sub>6</sub>H<sub>4</sub>, 224-5.5°, B, 60, alc.; Me, Me, H, p-MeC<sub>6</sub>H<sub>4</sub>, 225-7°, B, 74.7, alc.; Me, Me, H, 2,6-Et<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 218-18.5°, B, 48.5, alc.; Me, Me, H, NH<sub>2</sub>, 259-60°, B, 87.3, alc.; Ph, Me, H, H, 287-9°, A 82.5, alc., H<sub>2</sub>O; Ph, Me, H, Me, 162-3°, B, 80.2, alc., H<sub>2</sub>O; Ph, Me, Me, Me, 117-17.5°, C, 82.5, alc.; Ph, Me, H, Et, 86°, B, 87.2, alc.; Ph, Me, Et, Et, 66-8°, C, 83, alc.; Ph, Me, H, iso-Pr 143-4°, B 86, alc., H<sub>2</sub>O; Ph, Me, H, tert-Bu, 175-7°, C, 61, alc., H<sub>2</sub>O; Ph, Me, H, CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 159-60°, C, 49.1, C<sub>7</sub>H<sub>16</sub>; Ph, Me, CH<sub>2</sub>Ph, H, 187-8°, B, 92, alc.; Ph, Me, H, furfuryl, 153-4.5°, C, 56.2, PhMe, C<sub>7</sub>H<sub>16</sub>; Ph, Me, H, Ph, 262-3°, B, 50.5, EtOCH<sub>2</sub>CH<sub>2</sub>OH; Ph, Me, H, m-BrC<sub>6</sub>H<sub>4</sub>, 215-17°, B, 68, alc.; Ph, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>, 175-6°, B, 51.3, alc.; Ph, Me, H, m-ClC<sub>6</sub>H<sub>4</sub>, 192-3°, B, 90, alc.; Ph, Me, H, p-ClC<sub>6</sub>H<sub>4</sub>, 226-6.5°, B, 82, alc., H<sub>2</sub>O; Ph, Me, H, 2,6-Et<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 189-90°, B, 71.2, alc.; Ph, Me, H, NH<sub>2</sub>, 243-4°, B, 80.1, C<sub>5</sub>H<sub>5</sub>N; Ph, Me, H, NHPH, 240-1°, B, 47.5, C<sub>5</sub>H<sub>5</sub>N; Ph, Et, Me, Me, 90.5-1.0°, B, 55.5, alc.; Ph, Et, H, tert-Bu, 148-8.5°, C 73.3, alc. (sublimed); Ph, Et, H, CH<sub>2</sub>Ph, 129-9.5°, C, 48.5, C, 48.5, C<sub>6</sub>H<sub>6</sub>, alc.; Ph, Et, H, o-ClC<sub>6</sub>H<sub>4</sub>, 168-8.5°, B, 71.5, EtOCH<sub>2</sub>CH<sub>2</sub>OH; Ph, Et, H, m-ClC<sub>6</sub>H<sub>4</sub>, 187-9°, B, 74, alc.; Ph, Et, H, p-ClC<sub>6</sub>H<sub>4</sub>, 208.5-9.5°, B, 87.8, EtOCH<sub>2</sub>CH<sub>2</sub>OH; Ph, Et, H, o-MeC<sub>6</sub>H<sub>4</sub>, 175-6°, B, 75.5, alc.; Ph, Et, H, m-MeC<sub>6</sub>H<sub>4</sub>, 169.5°, B, 58, alc.; Ph, Et, H, p-MeC<sub>6</sub>H<sub>4</sub>, 199-200°, B, 78.6, alc.; Ph, Et, H, 2,5-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 181-3°, B, 42.1, alc.; Ph, Et, H, 2,6-Et<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 191-1.5°, B, 38, alc.; Ph, Et, H, NH<sub>2</sub>, 198-9°, B, 87.5, alc.; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, H, 296.5-8.0°, A, 75.7, alc.; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, Me, 181-2.5°, B, 86, MeOH, H<sub>2</sub>O; p-MeC<sub>6</sub>H<sub>4</sub>, Me, Me, Me, 149-51°, B, 82.2, alc.; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, Et, 144-6°, B, 80, alc., H<sub>2</sub>O; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 165°, C, 62.8, PhMe, C<sub>7</sub>H<sub>16</sub>; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>, 219-21°, B, 76.5, C<sub>5</sub>H<sub>5</sub>N; p-MeC<sub>6</sub>H<sub>4</sub>, Me, H, m-BrC<sub>6</sub>H<sub>4</sub>, 218-20°, B, 63.5, alc.; o-ClC<sub>6</sub>H<sub>4</sub>, Me, H, H, 294.5-9.5°, A, 71.8, alc.; o-ClC<sub>6</sub>H<sub>4</sub>, Me, Me, Me, 152-3°, C, 77.7, alc.; o-ClC<sub>6</sub>H<sub>4</sub>, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>, 196-8°, B, 63, alc.; p-BrC<sub>6</sub>H<sub>4</sub>, Me, Et, Et, 123-4°, B, 51.6, EtOCH<sub>2</sub>CH<sub>2</sub>OH, H<sub>2</sub>O; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, H, above 300°, A, 36, alc.; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, Me,

218-19°, B, 57.2, alc.; H<sub>2</sub>O; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, iso-PrO(CH<sub>2</sub>)<sub>3</sub>,  
 109-10°, B, 51.1, MeOH, H<sub>2</sub>O; p-ClC<sub>6</sub>H<sub>4</sub>, Me, (R<sub>4</sub>R<sub>5</sub> = ) (CH<sub>2</sub>)<sub>5</sub>,  
 127.5-8.5°, B, 61.3, alc., H<sub>2</sub>O; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, CH<sub>2</sub>Ph,  
 214°, B, 93.3, EtOCH<sub>2</sub>CH<sub>2</sub>OH; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, CH<sub>2</sub>CH<sub>2</sub>Ph,  
 175-6°, B, 60.1, alc.; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, o-ClC<sub>6</sub>H<sub>4</sub>,  
 221-2°, B, 62.0, C<sub>5</sub>H<sub>5</sub>N, p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, m-ClC<sub>6</sub>H<sub>4</sub>, 222-3°,  
 B, 85.5, EtOCH<sub>2</sub>CH<sub>2</sub>OH; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, p-ClC<sub>6</sub>H<sub>4</sub>, 239-9.5°, B, 88,  
 C<sub>5</sub>H<sub>5</sub>N; p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, m-BrC<sub>6</sub>H<sub>4</sub>, 230-2°, B, 74.2, C<sub>5</sub>H<sub>5</sub>N;  
 p-ClC<sub>6</sub>H<sub>4</sub>, Me, H, 2,5-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 200°, B, 71.5, EtOCH<sub>2</sub>CH<sub>2</sub>OH;  
 p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H, Me, 248-9°, B, 69, alc.; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, Me, Me,  
 196°, B, 51.2, alc., H<sub>2</sub>O; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H, iso-Pr, 190-2°,  
 B, 81.1, alc.; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H, Bu, 147°, B, 66.6, alc.;  
 p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, (R<sub>4</sub>R<sub>5</sub> = ) (CH<sub>2</sub>)<sub>5</sub>, 189-91°, B, 96, C<sub>5</sub>H<sub>5</sub>N; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>,  
 Me, H, CH<sub>2</sub>CH<sub>2</sub>NEt<sub>2</sub>, 145°, B, 91.7, alc., H<sub>2</sub>O; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H,  
 o-ClC<sub>6</sub>H<sub>4</sub>, 227-8°, B, 43.2, alc.; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Me, H,  
 p-ClC<sub>6</sub>H<sub>4</sub>, 278°, B, 87, AcOH. The ultraviolet spectra were given  
 for many of the compds. given above. The screening of these compds.  
 against tumors in mice thus far has not revealed any significant antitumor  
 agents in this series.



=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	142.36	324.61
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-19.20	-19.20

STN INTERNATIONAL LOGOFF AT 21:44:16 ON 25 MAR 2008